PB84-207554

EPA (Environmental Protection Agency) Environmental Modeling Catalogue Abstracts of Environmental Models

Systems Architects, Inc., Randolph, MA

Prepared for

Environmental Protection Agency, Washington, DC

Aug 82

U.S. Department of Commerce
National Technical Information Service
NTIS

United States
Environmental Protection
Agency

Information
Clearinghouse
Washington DC 20460

August 1982

PB84-207554

EPA

Environmental Modeling Catalogue

Abstracts of Environmental Models

REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U.S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

TECHNICAL REPORT DATA

(Please read Instructions on the reverse before completing)

1. REPORT NO.	2.	3. RECIPIENT'S ACCESSION NO. PB8 A 207554
4. TITLE AND SUBTITLE Environmental Modeling Catalogue - Abstracts of Environmental Models		5. REPORT DATE August 1982
		6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S)		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS Systems Architects, Inc.		10. PROGRAM ELEMENT NO.
		11. CONTRACT/~~GRANT NO.~~ XXXXXXX 68-01-4723
12. SPONSORING AGENCY NAME AND ADDRESS Management Information and Data Systems Division 401 M St., S.W. Washington, D.C. 20460		13. TYPE OF REPORT AND PERIOD COVERED
		14. SPONSORING AGENCY CODE EPA 400/03

15. SUPPLEMENTARY NOTES

16. ABSTRACT

The Environmental Modeling Catalogue represents a part of EPA's efforts to establish communication and share information among researchers interested in modeling applications and techniques.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group

18. DISTRIBUTION STATEMENT	19. SECURITY CLASS *(This Report)*	21. NO. OF PAGES 419
	20. SECURITY CLASS *(This page)*	22. PRICE

EPA Form 2220-1 (Rev. 4-77) PREVIOUS EDITION IS OBSOLETE

EPA ENVIRONMENTAL MODELING CATALOGUE

Prepared for

EPA Information Clearinghouse (PM-211A)
Library Systems and Services Staff
U.S. Environmental Protection Agency
401 M Street, SW
Washington, DC 20460

August 1982

1-a

FOREWARD

A substantial amount of current environmental analysis employs mathematical modeling techniques. This publication, EPA Environmental Modeling Catalogue, represents a part of EPA's effort to establish communication and share information among researchers interested in modeling applications and techniques.

The EPA has made a commitment to support environmental modeling in various forms. Two significant efforts have been made in the areas of water quality and air quality. The Center for Water Quality Modeling was established by the Office of Research and Development as a central service activity where users can obtain models and instructions in their use*. Tom Barnwell is the chief of this center. Air quality models are developed and supported through the Environmental Operations Branch located at the Research Triangle Park in North Carolina. D. Bruce Turner is the chief of this Branch and has primary responsibility for air quality modeling efforts (He can be reached at FTS 629-4564 or 919/541-4564). Other attempts to promote mathematical modeling involve EPA sponsorship of modeling conferences. These include "Environmetrics '81'", a conference on statistical and mathematical methodologies applied to problems in environmental quality, and "EPA Conference on Environmental Modeling and Simulation," held in Cincinnati, Ohio in April of 1976.

This document was developed by Systems Architects, Inc. under Task No. 12 to EPA Contract No. 68-01-4723. The EPA Project Officer was Elijah Poole of the Management Information and Data Systems Division.

*Services are available by dialing (404)546-3585, FTS 250-3585 or writing the Center for Water Quality Modeling, Environmental Research Laboratory, USEPA, College Station Road, Athens, GA 30613.

ACKNOWLEDGEMENTS

The major support for this second edition of the EPA Environmental Modeling Catalogue came from the numerous sources both within and outside of EPA who contributed abstracts of environmental models. As this catalogue contains abstracts of some 103 models, there are too many names to acknowledge individually in this section. However, we want to give special thanks to Martha McDonald, former Director of the Information Clearinghouse and members of her staff, Harvey Karch and Deborah Ranciato, for conducting a survey of models. This survey provided information on numerous additional models. Finally, we want to thank Tom Barnwell and Bruce Turner for performing peer review and providing editorial comments.

TABLE OF CONTENTS

INTRODUCTION	---	ix

AIR QUALITY MODELS

Air Pollution Research Advisory Committee Model 1A	APRAC-1A	1
Air Pollution Research Advisory Committee Model 2	APRAC-2	6
Air Quality Display Model	AQDM	13
Averaging Time Model	AVGTIME	16
Climatological Dispersion Models	CDMQC, CDM	20
Gaussian Plume Dispersion Algorithm	VALLEY	25
Gaussian Plume Multiple Source Air Quality Algorithm	RAM	31
HIWAY Model	HIWAY	38
HIWAY-2	HIWAY-2	42
Industrial Source Complex Model	ISC	46
Kinetic Model and Ozone Isopleth Plotting Package	OZIPP	50
Lagrangian Photochemical Air Quality Simulation Model	LPAQSM	54
Livermore Regional Air Quality Model	LIRAQ	56
Modified Rollback Model	ROLLBACK	60
Multiple Point Gaussian Dispersion Algorithm with Optional Terrain Adjustment	MPTER	63
Multi-Source Model	CRSTER-2	66
Nonlinear Rollback/Rollforward Model	---	68
The Plume Visibility Model	PLUVUE	70
Point, Area, Line Source Algorithm	PAL	74
Point Source Gaussian Plume Model	PTPLU	78
Point Source Models	PTMAX, PTDIS & PTMTP	81

AIR QUALITY MODELS (Continued)

Reactive Plume Model RPM-II 86
Regional Emissions Projection System REPS 90
SAI Airshed Model SAIASP 93
Simulation of Human Air Pollution Exposures SHAPE 97
Single Source Model CRSTER 103
Systems Applications, Inc. Model SAI 108
Texas Climatological Model Version 2 TCM-2 111
Texas Episodic Model Version 8 TEM-8 116

ECONOMIC MODELS

Abatement and Residual Forecasting Model ABTRES 120
Air Test Model AIRTEST 123
Automobile Demand Model CARMOD 125
Construction Model CONMOD 132
Section 120 Noncompliance Penalty Model PENALTY 135
Steel Industry Model PTM 138
Strategic Environmental Assessment System SEAS 144
U.S. Copper Industry Model COPMOD1 151

NOISE MODELS

Construction Site Health and Welfare CSM 154
National Roadway Traffic Noise Exposure Model --- 157
Railroad Health and Welfare Model RMEA 79N3 159

OTHER MODELS

A Mathematical Model for Fast- Screening Procedure for Testing the Effects of Pollutants in Mammals	---	161
Premixed One-Dimensional Flame Code	PROF	165
Waste Resource Allocation Program	WRAP	168

RADIATION MODELS

Atmospheric Dispersion of Radionuclides	AIRDOS-EPA	173
Great Lakes Dose/Concentration	GLA-1	177
High Level Radioactive Waste Repository Risk Model	REPRISK	179
Maximum Individual Dose Model	MAXDOSE	182
Nonionizing Radiation Models	---	184
Plutonium Air Inhalation Dose	PAID	189
Radionuclide Dose Rate/Risk	RADRISK	191

TOXIC SUBSTANCES MODELS

A Computer Program For The Risk Assessment of Toxic Substances	MULTI80G	195
Environmental Partitioning Model	ENPART	198
Exposure Analysis Modeling System	EXAMS	201
A FORTRAN Program for Risk Assessment Using Dose-Response Data Time-To Occurence	RANK TIME	212
A FORTRAN Program to Extrapolate Dichotomous Animal Carcinogenicity Data to Low Doses	GLOBAL 79	215
Mantel-Bryan Low-Dose Extrapolation Model	MANTELAN	218
One-Hit Low-Dose Extrapolation Model	ONE HIT MD	221
Seasonal Soil Model	SESOIL	224

TOXIC SUBSTANCES MODELS (Continued)

Statistical Methodology for Toxicological Research	MRST	227
Unified Transport Model - Toxics	UTM-TOX	230
Urban Wastewater Toxics Flow Model	TOXFLO	233

WATER QUALITY MODELS

Centralized Treatment of Industrial Wastewater	---	236
Computer Program for Chemical Equilibria in Aqueous Systems	REDEQL.DWRD	241
Computer Program for Chemical Equilibria in Aqueous Systems	REDEQL.EPAK	245
Dissolved Oxygen Sag Model	DOSAG-I	250
Dynamic Estuary Model	DEM	254
Enhanced Hydrodynamical - Numerical Model for Near Shore Processes	HN	259
Estuarine Water Quality Model	ES001	263
EXEC/OP Version 1.2	EXEC/OP	266
Georgia Dosag	GADOSAG	270
Hydrological Simulation Program-FORTRAN	HSPF	272
LAKE-I Ecologic Model	LAKE-I	282
Level III - Receiving Water Quality Modeling for Urban Stormwater Management	---	285
M.I.T. Transient Water Quality Network	---	289
Multi- Segment Comprehensive Lake Ecosystem Analyzer for Environmental Resources	MINI.CLEANER	295
National Residuals Discharge Inventory	NRDI	302
Outfall Plume Model	PLUME	307
Receiving Water Model	DIURNAL	311
Receiving Water Model	RECEIV-II	314
Receiving Water Quality Model	RWQM	318
River Basin Model	RIBAM	321

WATER QUALITY MODELS (Continued)

River Temperature Simulation Model	TEMPSTAT	324
Simplified Estuary Model	SEM	327
Simplified Stream Model	SSM	330
Stream 7B	STREAM 7B	333
Stream Network Simulation Program	SNSIM	335
Stream Quality Model	QUAL-II	338
Tidal Temperature Model	TTM	342
Time-Dependent, Three-Dimensional Transport Model	---	345
Time-Dependent, Three-Dimensional, Variable-Density Hydrodynamic Model	---	348
Water Quality Assessment Methodology for Toxic and Conventional Pollutants	WQAM	353
Water Quality Feedback Model	FEDBAK03	356
Water Quality for River - Reservoir Systems	WQRRS	358
Water Quality Model	EXPLORE-I	363
Water Quality Model	HAR03	367
Water Quality Modeling System for the Great Lakes	WQMSGL	371

WATER RUNOFF MODELS

Agricultural Runoff Model Version II	ARM II	377
Agricultural Watershed Runoff Model	AGRUN	383
Non Point Source Pollutant Loading Model	NPS	386
One-Dimensional Groundwater Mass Transport Model	GWMTM1	391
Storage, Treatment, Overflow, Runoff Model	STORM	393
Storm Water Management Model (Version III)	SWMM	398
Two-Dimensional Groundwater Mass Transport Model	GWMTM2	408

INTRODUCTION

The Environmental Protection Agency was established in 1970 to provide a focal point at the national level for monitoring and improving the Nation's environment. An important element of this mission is the use of analysis and research aimed at identifying, quantifying, and providing solutions to environmental problems. Modeling techniques are a cost effective and widely applicable tool in the performance of EPA research. Computers assist immeasurably in this area since they are an effective means for applying most modeling techniques.

The objective of this catalogue is to provide a reference to existing modeling applications in a variety of subject areas. These subjects include water quality, water runoff, air quality, toxic substances, noise, radiation and economics. It is hoped that this reference will promote communication and resource sharing among the various groups conducting environmental research.

This publication is the second in a series of Environmental Modeling Catalogues. Each model is described by an abstract that was provided by the technical contact. Each abstract contains the following components: Model Overview, Functional Capabilities, Basic Assumptions, Input and Output, System Resource Requirements, Applications, Technical Contact(s), and References. Each abstract will permit an evaluation of the model's applicability to the reviewer's research area.

Additional models or enhancements to the descriptions contained in this catalogue should be forwarded to the Environmental Protection Agency, Management Information and Data Systems Division, PM-218, 401 M Street, S.W., Washington, D.C. 20460.

AIR POLLUTION RESEARCH ADVISORY COMMITTEE
MODEL 1A (APRAC-1A)

1. Model Overview: APRAC, Stanford Research Institute's urban carbon monoxide model, computes hourly averages for any urban location. The model requires an extensive traffic inventory for the city of interest, and its requirements and technical details are documented in User's Manual for the APRAC-1A Urban Diffusion Model Computer Program, which is available from NTIS.

2. Functional Capabilities: The computer program can be used to make calculations of the following types:

- Synoptic model: hourly concentrations as a function of time, for comparison and verification with observed concentrations and for operational application.
- Climatological model: the frequency distribution of concentrations, for statistical prediction of the frequency of occurence of specified high concentrations in connection with planning activities.
- Grid-point model: concentrations at various locations in a geographical grid, providing detailed horizontal concentration patterns for operational or planning purposes.

Roadway link information is limited to 1200 sources.

3. Basic Assumptions:

A. Source-Receptor Relationship. The user specifies the set of traffic links (line sources) by providing link endpoints, road type and daily traffic volume. The traffic links may have arbitrary length and orientation. Off-link traffic is allocated to a 2 x 2 mi. grid. Link traffic emissions are aggregated into a receptor oriented area source array. The boundaries of the area sources actually treated are:1) arcs at radial distances from the receptor which increase in geometric progression; 2) the sides of a 22.5° sector oriented upwind for distances greater than 1000 m.; and 3) the sides of a 45° sector oriented upwind for distances less than 1000 m. A similar area source array is established for each receptor. Sources are assumed to be at ground level, and up to ten receptors are allowed in the model. Receptors are at ground level and their locations can be arbitrary. Four internally defined receptor locations on each user-designated street are used in a special street canyon sub-model.

B. Emission Rate. Daily traffic volume for each link and off-link grid square is input and modified by various factors to produce hour-by-hour emissions from each link. Link emissions are aggregated as described above: sector area source contributions are obtained analytically. Off-link traffic emissions on a two mile grid square are added into the sector area sources. In the street canyon sub-model, a separate hourly emission rate is provided by the user for the link in question.

C. Plume Behavior. The model does not treat plume rise, and it does not treat fumigation or downwash except in the street canyon sub-model. In the street canyon sub-model, a helical circulation pattern is assumed.

D. Horizontal Wind Field. Input for the model is hourly wind speed and direction in tens of degrees. No variation of wind speed or direction with height is allowed. A constant, uniform (steady-state) wind is assumed within each hour.

E. Vertical Wind Speed. This is assumed to be equal to zero except in the street canyon sub-model, where a helical circulation pattern is assumed.

F. Horizontal Dispersion. Section averaging has a uniform distribution within sectors. Each section larger than 1 km. is divided into sectors of 22.5°; sections within 1 km. of size are divided into sectors of 45°.

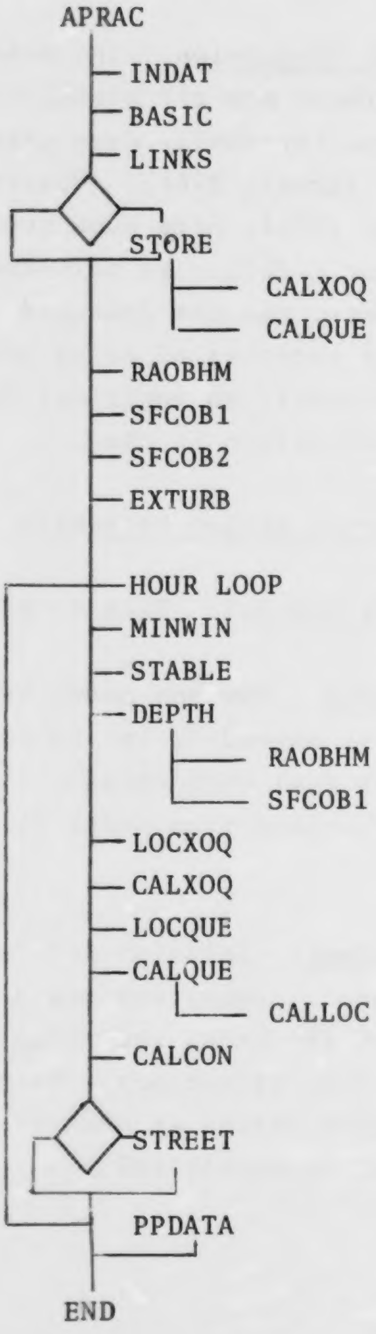
G. Vertical Dispersion. The model utilizes a semi-empirical/Gaussian plume. There are six stability classes, and each stability class is determined internally from user-supplied meteorological data (modified by Turner, 1964). Dispersion coefficients from McElroy and Pooles (1968) have been modified using information in Leighton and Ditmar (1953). No adjustments are made for variations in surface roughness, and the downwind distance variation of σ_z is assumed to ax^b for purposes of doing analytic integration. In the street canyon sub-model, an empirical function of wind speed and street width and direction is used.

H. Chemistry/Reaction Mechanism. This is not treated.

I. Physical Removal. This is not treated.

J. Background. The box model used to estimate contributions from upwind sources beyond 32 km. is based on wind speed, mixing height, and annual fuel consumption. In the street canyon sub-model, contributions from other streets are included in the background.

4. Input and Output: Emission and meteorological information are needed for the model. Emissions are a function of the hour of the day and the day of the week, and meteorological parameters are functions of the hour of the day. Output from the model includes hourly concentration values at each receptor and frequency distribution based on hourly values.


APRAC
INDAT
BASIC
LINKS
STORE
CALXOQ
CALQUE
RAOBHM
SFCOB1
SFCOB2
EXTURB
HOUR LOOP
MINWIN
STABLE
DEPTH
RAOBHM
SFCOB1
LOCXOQ
CALXOQ
LOCQUE
CALQUE
CALLOC
CALCON
STREET
PPDATA
END

FLOWCHART FOR APRAC 1A

5. System Resource Requirements: The dispersion model is written in FORTRAN V. The program does not require any special software or utilities. Approximately 32K of core memory is required to execute on the Univac 1110.

6. Applications: The source program for this dispersion model is available as part of UNAMAP (Version 3), PB 277 193, for $420 from Computer Products, NTIS, Springfield, VA 22161.

7. Technical Contact

D. Bruce Turner
U.S. Environmental Protection Agency
Mail Drop 80
Environmental Applications Branch
Research Triangle Park
NC 27711

FTS 629-4564 COM 919/541-4564

8. References

Dabbert, W.F., Ludwig, F.L., and Johnson, W.B., Jr., "Validation and Applications of an Urban Diffusion Model for Vehicular Pollutants", *Atmos. Environ.*, 7, 603-618, 1973.

Evaluation of the APRAC-1A Urban Diffusion Model for Carbon Monoxide, NTIS Accession Number PB 210-813.

Field Study for Initial Evaluation of an Urban Diffusion Model for Carbon Monoxide, NTIS Accession Number PB 203-469.

Johnson, W.B., Ludwig, F.L., Dabbert, W.F., and Allen, R.J., "An Urban Diffusion Simulation Model for Carbon Monoxide", *Journal of the Air Pollution Control Association*, 23, 6, pp. 490-498, 1973.

A Practical, Multipurpose Urban Diffusion Model for Carbon Monoxide, NTIS Accession Number 196-003.

User's Manual for the APRAC-1A Urban Diffusion Model Computer Program, NTIS Accession Number PB 213-091 (@ $5.25 per paper copy, $2.25 for microfiche).

AIR POLLUTION RESEARCH ADVISORY COMMITTEE MODEL 2 (APRAC-2)

1. Model Overview: The APRAC-2 model is a revised version of the APRAC-1A diffusion model. It maintains basically the same approach to the simulation of atmospheric diffusion, but it incorporates recent advances in the estimation of vehicular emission and in the dissemination of traffic information. One of the most important characteristics of the APRAC-2 model is its ability to make full use of the historic records and the projections available from the Federal Highway Administration`s (FHWA) battery of computer programs. Mixing depth information from alternative sources can be used. The model now can provide as outputs the amount of pollutant emitted in grid squares through the area. The APRAC-2 model uses EPA`s emissions calculation methodology from Supplement No. 5 to AP-42.

2. Functional Capabilities: The model has two major components: A diffusion module (DIFMOD), and an emission module (EMOD). The emissions module can operate without the diffusion module, but the diffusion model requires the outputs from the emissions module as its inputs. Each of the two modules has several major components. The emissions module has components to calculate tables of emissions, a component to determine emissions on each roadway link, and a component that estimates the emissions within each grid square.

The three major functions of the diffusion model are to: (1) calculate diffusion; (2) derive, from conventional meterorological information the stability, mixing depth, and wind parameters used by the model; and (3) simulate small-scale effects near the receptor. Diffusion calculations can be made for as many as 625 locations for a single hour and as many as 10 locations for a single day or for a year at a single station. There are two subroutines in the small-scale effects category: one treats canyon conditions and the other simulates traffic and dispersion in the vicinity of an intersection.

ARPAC-2 can treat hydrocarbons, carbon monoxide, or oxides of nitrogen. Diffusion calculations make use of a receptor-oriented Gaussian plume model. Local winds at the receptor can be used, and they are interpolated from multiple wind inputs. Mixing heights may be calculated from sounding data, or input directly. A small program is included from decoding Federal Highway Administration data tapes.

3. Basic Assumptions: The method utilized by APRAC-2 for computing emission factors has been described in detail by Kircher and Williams (1975). Percentages of vehicles operating in cold, hot transient, and hot stabilized modes are assumed to vary with time of day and from one part of a city to another. If land use categories are not specified, the model assumes that all central business district area types correspond to the same locale type. Core city areas are assumed to be commercial. Suburban streets are assumed to be commercial if their average weekday traffic exceeds 10,000; otherwise the locale is taken to be residential. The locale for areas that do not fit specified categories is taken to be rural or unclassified.

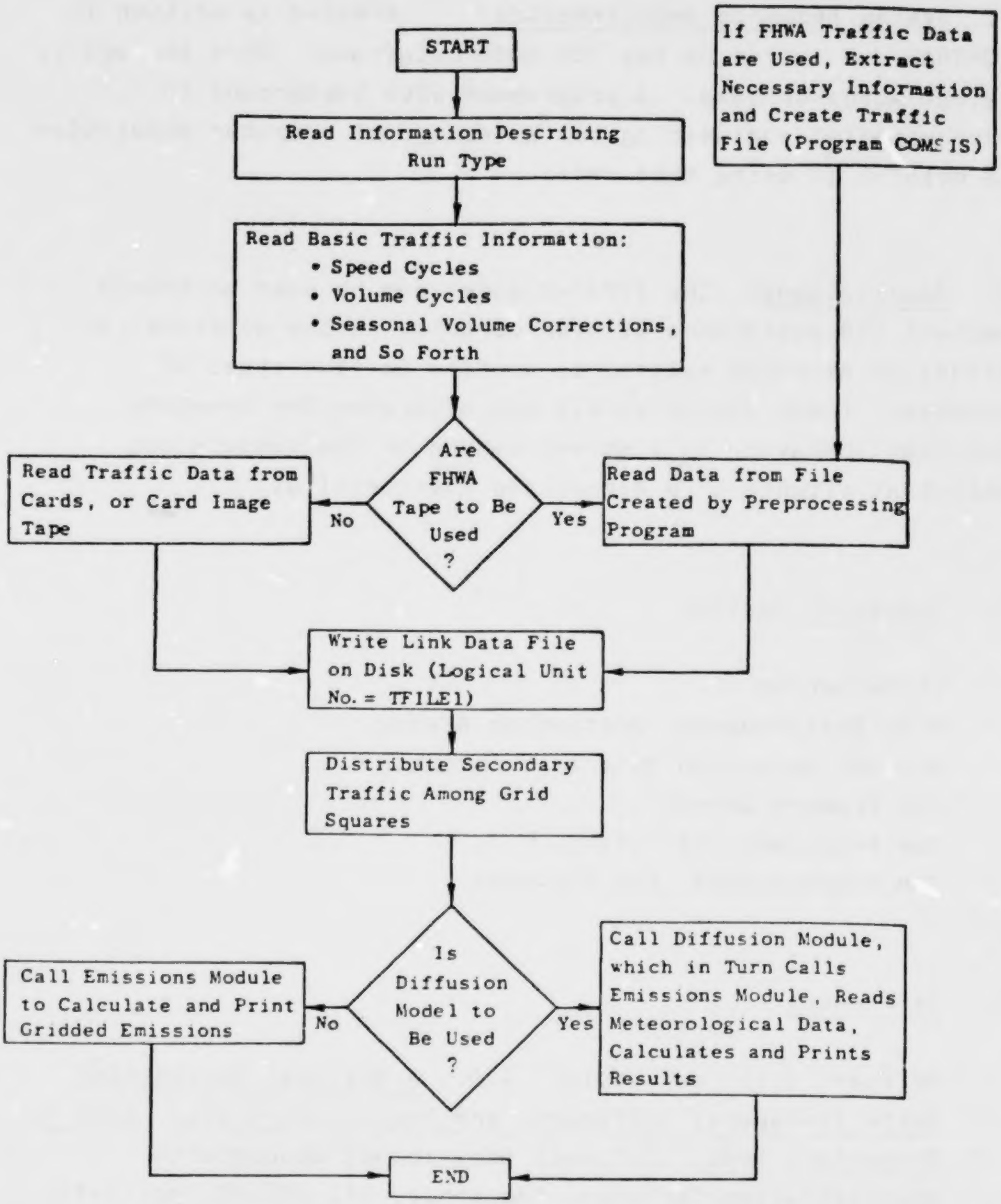
A Gaussian-plume diffusion formulation is used for diffusion calculations. The model uses an atmospheric stability algorithm derived by Ludwig and Dabbert (1976) from the basic method proposed by Pasquill (1961). Daytime stability categories are based on wind speed and the strength of the incoming solar radiation.

4. Input and Output: If FHWA traffic data are to be used, they must first be converted to a format compatible with the rest of the program. For IBM machines this is done with the program COMSIS, which will read and unpack the data and then create a file for subsequent use by the APRAC-2 program.

The input required to operate the EMOD module is as follows: the first 17 cards are all required to identify which options are to be used during the run and the other parameters that define the nature of the run. The next 72 cards define the diurnal traffic cycles appropriate to different kinds of roadway, areas of the city, and days of the week.

At least 22 cards are required to operate the DIFMOD model. The first six cards are required to define the region, the types of calculations to be made, and the coordinates of the receptors in kilometers with the origin at the same place as the emissions grid. Cards D-6 through D-9 define the length of the run, street canyon features, intersection link features and coordinates, holidays, and pollutants to be treated. Cards D-10 through D-15b define upwind background concentrations; mixing depth input type; station, date, maximum and minimum temperatures, and daylight savings time; radiosonde data, weather data, and wind data for up to 100 sites; intersection traffic parameters; and intersection signalization parameters.

Output provided by the model includes computer printouts of ambient air concentration for hydrocarbons, carbon monoxide, or oxides of nitrogen as amounts of pollutant emitted in grid squares throughout the area; and a listing of the input data.


START
Read Information Describing Run Type
Read Basic Traffic Information:
• Speed Cycles
• Volume Cycles
• Seasonal Volume Corrections, and So Forth
If FHWA Traffic Data are Used, Extract Necessary Information and Create Traffic File (Program COMSIS)
Are FHWA Tape to Be Used ?
No
Yes
Read Traffic Data from Cards, or Card Image Tape
Read Data from File Created by Preprocessing Program
Write Link Data File on Disk (Logical Unit No. = TFILE1)
Distribute Secondary Traffic Among Grid Squares
Is Diffusion Model to Be Used ?
No
Yes
Call Emissions Module to Calculate and Print Gridded Emissions
Call Diffusion Module, which in Turn Calls Emissions Module, Reads Meteorological Data, Calculates and Prints Results
END

SIMPLIFIED FLOWCHART FOR APRAC II

5. System Resource Requirements: APRAC-2 is written in FORTRAN and is run on the CDC 6400 mainframe. Core storage is 55,000 words or less. A programmer with background in environmental engineering and knowledge of computer simulation is helpful in using this model.

6. Applications: The APRAC-2 model can be used to assess ambient concentrations of hydrocarbons, carbon monoxide, or oxides or nitrogen emitted by traffic in five types of locales. Local source models are available for treating pollutant behavior in a street canyon or the vehicle and pollutant effects at a signalized intersection.

7. Technical Contact

Linda Larson
U.S. Environmental Protection Agency
Air and Hazardous Materials Division
215 Fremont Street
San Francisco, CA 94105
COM 415/556-2004 FTS 556-2004

8. References

Heffter, J.L., and Taylor, A.D., A Regional Continental Scale Transport, Diffusion, and Deposition Model. Part I: Trajectory Model, National Oceanic and Atmospheric Administration Technical Memoranda, ERL ARL-50, pp. 1-16, 1975.

Johnson, W.B., Dabberdt, W.F., Ludwig, F.L., and Allen, R.J., Field Study for Initial Evaluation of an Urban Diffusion Model for Carbon Monoxide, Comprehensive Report CRC and Environmental Protection Agency, Contract CAPA-3-68 (1-69), 1971.

Kircher, D.S. and Williams, M.E., Supplement No. 5 for Compilation of Air Pollutant Emission Factors (AP-42), Chapter 3 (second edition), U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, (OAQPS), 1975.

Kunselman, R., McAdams, H.T., Domke, C.J., and Williams, M., Automobile Exhaust Emission Modal Analysis Model, EPA Contract 68-01-0438, Calspan Corporation, Buffalo, New York, 1974.

Ludwig, F.L., "Urban Air Temperatures and Their Relation to Extra-Urban Meteorological Measurements," Proceedings of the Semi-annual Meeting of the American Society of Heating, Refrigeration, and Air Conditioning Engineers, (Survival Shelter Problems, Part II) San Francisco, pp. 40-45, January 1970.

Ludwig, F.L. and Dabberdt, W.F., Evaluation of the APRAC1A Urban Diffusion Model for Carbon Dioxide. Final Report, CRC and EPA Contract CAPA-3-68 (1-69), 1972.

Ludwig, F.L. and Dabberdt, W.F., "Comparison of Two Atmospheric Stability Classification Schemes in an Urban Application," Journal of Applied Meteorology, 15, 11721176, 1976.

Ludwig, F.L., Johson, W.B., Moon, A.E., and Mancuso, R.L., A Practical, Multipurpose Urban Diffusion Model for Carbon Monoxide. Final Report, Coordinating Research Council (CRC), Contract CAPA-3-68 and National Air Pollution Control Administration Contract CPA 22-69-64, 1970.

Ludwig, F.L. and Kealoha, J.H.S., Selecting Sites for Carbon Monoxide Monitoring, Final Report, EPA Contract 68-02-1471, Stanford Research Institute, Menlo Park, Califonia, 1975.

Mancuso, R.L. and Ludwig, F.L., User's Manual for the APRAC-1A Diffusion Model Computer Program, CRC and EPA, Contract CAPA-3-68(1-69), 1972.

Sagi, G. and Campbell, L., "Vehicle Delay at Signalized Intersections," Traffic Engineering, 1969.

Sandys, R.C., Buder, P.A., and Dabberdt, W.F., ISMAP: A Traffic/Emissions/Dispersion Model for Mobile Pollution Sources, prepared for the California Business Properties Association, Hawthorne, Califonia, by the Stanford Research Institution, Menlo Park, California, 1975.

U.S. Department of Transporation, Federal Highway Administration, Urban Transporation Planning, General Information, 1972.

AIR QUALITY DISPLAY MODEL (AQDM)

1. Model Overview: The Air Quality Display Model (AQDM) is a three-dimensional, steady-state air model used in the evaluation of area sources in "rough" urban areas. The AQDM treats the physical processes of both transport and diffusion. The model is appropriate for examining areas ranging in size from small localized vicinities to whole urban areas, and it has a long-term application for the evaluation of seasonal or annual air quality variations.

2. Functional Capabilities: The AQDM model does not simulate chemical processes, but it does treat the physical processes of transport and diffusion in "rough" urban areas. It uses a one layer discretization and a user-specified 14 x 14 grid. A 225 grid receptor with 12 additional receptor points is also user-specified. The fixed-point meteorological data does not describe micrometeorological variations within the city, nor does it describe "urban heat island" air circulations. The model has a sensitivity to effective stack height, wind speed, and wind stability. It is limited to SO_2 and suspended particulates, and it is designed for annual average and seasonal applications.

3. Basic Assumptions: The AQDM is a deterministic model that uses an analytically integrated solution technique. It assumes a steady state for air quality constituents, Gaussian diffusion, and homogeneous, discrete atmospheric conditions.

4. Input and Output: Input to the model for initial set-up and calibration include: point and area residual discharges and stack parameters which consist of height, diameter, temperature, and exit velocity; meteorological data containing wind speed and direction, stability, and mixing height; and several ambient air concentration measurements. Model data requirements for verification incorporate the above meteorological data and ambient air concentration measurements.

Output for the model includes ambient concentration values given at grid locations, ground level, or other user-selected points. These values are given in the form of tabular printouts or card decks for use with CALCOMP or SYMAP plot programs. Some of the special features of the AQDM output are its statistical output routines, receptor contribution analysis, and calibration subroutines.

5. System Resource Requirements: AQDM is coded in FORTRAN and is run on an IBM 360/40 or an equivalent system. It requires 300K bytes of core memory for execution. A background in programming and engineering is useful.

6. Applications: AQDM can be used in the evaluation of area sources in "rough" urban areas for seasonal or annual air quality variations. This model has been superceded by such models as CDM/CDMQC and RAM; thus AQDM is primarily of historical interest.

7. Technical Contact

Joe Tikvart
U.S. Environmental Protection Agency
Monitoring and Data Analysis Division
Mutual Building
411 W. Chapel Hill St.
Durham, N.C. 28801
COM 919/541-5561 FTS 629-5561

8. References

Croke, I.E., *et al.*, "Regional Implementation Plan Evaluation Process," ANC/ES-DA-001, Argonne National Laboratory, Argonne, Illinois, (July 1970).

National Air Pollution Control Administration, "Air Quality Display Model," PB 189 194, Washington, D.C., (November 1969).

AVERAGING TIME MODEL (AVGTIME)

1. Model Overview: AVGTIME is a mathematical model based on two characteristics that are often demonstrated by air-quality data: (1) air pollutant concentrations tend to be lognormally distributed (Figure 1) for all averaging times and (2) median (50 percentile) concentrations tend to be proportional to averaging time raised to an exponent and thus plot as a straight line on logarithmic graph paper (Figure 2). Two percentile concentrations (at the same or at different averaging times) are read into the model and concentrations for the maxima or any percentiles can then be calculated for any other averaging times.

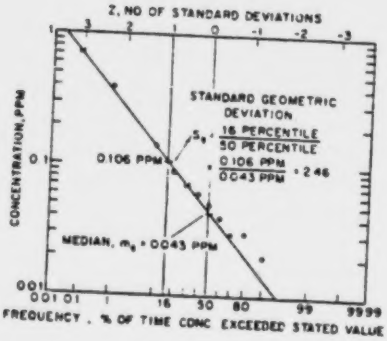


Figure 1. Frequency that various 1-hr-averaging-time nitrogen oxides concentrations exceeded various values in Washington D.C. from 12/1/61 to 12/1/64

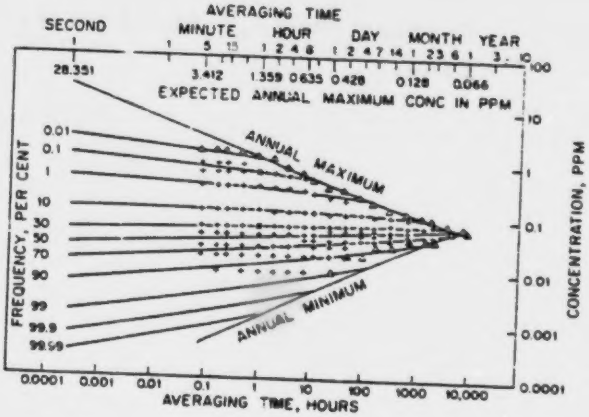


Figure 2. Concentration vs. averaging time and frequency for nitrogen oxides in Washington from 12/1/61 to 12/1/64

2. Functional Capabilities: The detailed characteristics of the model are described by a dozen equations on pp. 51-52 in Ref. 2. Two input concentrations are entered into the proper equation to calculate two output parameters: the geometric mean and standard geometric deviation for one averaging time. The other equations are then used to calculate these two output parameters, the maxima, and the concentrations for any desired percentiles for any other averaging times.

3. Basic Assumptions: Analyses of air pollutant concentration data suggest that urban concentrations often tend to fit a general mathematical model having the following three characteristics:

1) Pollutant concentrations are lognormally distributed for all averaging times.

2) Median concentrations are proportional to averaging time raised to an exponent.

3) Maximum concentrations are approximately inversely proportional to averaging time raised to an exponent.

A 2-parameter averaging time model with the above three characteristics has been developed.

Air pollutant concentrations measured near isolated point sources often do not fit a 2-parameter lognormal distribution very well. Such data often do fit a 3-parameter lognormal distribution fairly well. A 3-parameter averaging time model has therefore been developed to model such data.

4. Input and Output: The user inputs any two air quality measurements for the 2-parameter model. These two input parameters might be, for instance, the concentrations exceeding

0.1% and 30% of the time for 1-hour average concentrations. The two input concentrations can be at the same or at different averaging times. The user inputs any three air quality measurements into the 3-parameter model, at either the same or at different averaging times.

The equations mentioned under "Functional Capabilities" are used to calculate expected concentrations. Expected highest and second highest concentrations for various averaging times (1, 3, 8, and 24 hr, and 1 year) can be easily determined by using Table II in Ref. 3.

The 3-parameter averaging time model is more difficult to use than is the 2-parameter model. Trial and error techniques can be used to calculate the third parameter (a constant that is added or subtracted from each of the three input concentration measurements) needed to fit the data to a 2-parameter lognormal distribution.

5. System Resource Requirements: AVGTIME is coded in FORTRAN and is run on an Univac 1100 or any equivalent mainframe computer. It requires 40K bytes of core memory for execution. Operation needs include a background in environmental engineering and air quality. A 500 card FORTRAN job deck is available that will calculate expected maxima and percentile concentrations for several averaging times based on three concentration measurements input to the model. The job deck is available on request from the Technical Contact .

6. Applications: As the title of Ref. 2 implies, the averaging time model has been used to relate air quality measurements to air quality standards to determine overall average percent emission reductions needed to achieve air quality standards. The input air quality data can either be measured or dispersion-modeled.

Air quality data for one averaging time has been used to calculate percentiles and expected maxima for other averaging times for which air quality standards have been written. Air quality measurements might be available for 24-hour average concentrations of sulfur dioxide for instance. The model could be used to calculate expected maximum concentrations for 3-hour averages and these maxima could then be compared with the 3-hour sulfur dioxide National Ambient Air Quality Standard (NAAQS).

7. Technical Contact

Ralph I. Larson
U.S. Environmental Protection Agency
Environmental Science Research Laboratory
Mail Drop 80
Research Triangle Park
N.C. 27711
COM 919/541-4564 FTS 629-4564

8. References

Larsen, R.I., "A New Mathematical Model of Air Pollutant Concentration, Averaging Time, and Frequency", Journal of the Air Pollution Control Assoc., 19 (1), 24-30, 1969.

Larsen, R.I., A Mathematical Model for Relating Air Quality Measurements to Air Quality Standards, Publ. AP-89, U.S. Environmental Protection Agency, Research Triangle Park, NC, 56 pp., 1971.

Larsen, R.I., "An Air Quality Data Analysis System for Interrelating Effects, Standards, and Needed Source Reductions: Part 4. A Three-Parameter Averaging-Time Model," Journal of the Air Pollution Control Assoc., 27 (5), 454-459, 1977.

CLIMATOLOGICAL DISPERSION MODELS (CDMQC, CDM)

1. Model Overview: The Climatological Dispersion Models (CDMQC, CDM) determine long-term (seasonal or annual) quasi-stable pollutant concentrations at any ground level receptor using average emission rates from point and area sources and a joint frequency distribution of wind direction, wind speed, and stability for the same period. The User's Guide for the Climatological Dispersion Model describing the CDM is available from NTIS (accession number PB 227-346-AS). The Addendum to User's Guide for Climatological Dispersion Model describing the enhancements available in the CDMQC is available from EPA as EPA-45013-77-015 and from NTIS (PB-274-040).

2. Functional Capabilities: Long-term concentrations corresponding to the period of joint frequency distribution of meteorological data (usually seasonal or annual) are produced for each receptor, assuming that the emission inventory is valid for the same period. The two contributions to the concentration, those due to points and those due to areas, are output. Receptor locations are specified by the user. An option is available to produce a pollutant rose-contribution to the total concentration from each direction.

3. Basic Assumptions:

A. Source-Receptor Relationship. CDMQC and CDM use an arbitrary location for each point source, and area sources are represented in uniform grid squares. Receptor locations are arbitrary, as are release heights for point and area sources. Receptors are assumed to be at ground level. The model assumes that there are no terrain differences between the sources and receptors.

B. Emission Rate. A single rate is allowed for each point and area source. For area sources, area integrations are done numerically, one 22.5^{o} sector at a time; sampling at discrete points is defined by specific radial and angular intervals on a polar grid centered on the receptor.

C. Chemical Composition. CDMQC and CDM treat one or two pollutants simultaneously.

D. Plume Behavior. Only Briggs (1971) neutral/unstable formula is used by the model. If the stack height plus the plume rise is greater than the mixing height, then the ground level concentrations are assumed to be equal to zero. As an alternate to the Briggs formula, the input value of the plume rise times the wind speed for each point source can be used. No plume rise is calculated for area sources. CDMQC and CDM do not treat fumigation or downwash.

E. Horizontal Wind Field. The models use a climatological approach, and utilizes 16 wind directions and 6 wind speed classes. The wind speed is corrected for the release height based on the power law variation exponents from DeMarrais (1959). A constant, uniform (steady-state) wind is assumed.

F. Vertical Wind Speed. This is assumed to be equal to zero.

G. Horizontal Dispersion. The models use a climatological approach, and assume a uniform distribution within each of 16 sectors (narrow-plume approximation). Averaging time for the model is one month to one year.

H. Vertical Dispersion. The models use a semi-empirical/ Gaussian plume with five stability classes as defined by Turner

(1964). Neutral stability is split into day/night cases on input, and dispersion coefficients are taken from Turner (1970). The stability classes for area sources are decreased by one category from the input values (to account for urban effects). Neutral dispersion coefficients are used for all neutral and stable classes. No provision is made for variations in surface roughness.

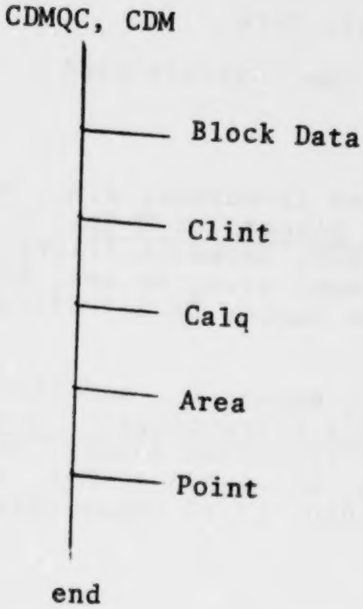
I. Chemistry/Reaction Mechanism. The models use exponential decay and a user-input half-life.

J. Physical Removal. The model utilizes exponential decay and a user-input half-life. The same rate constant is always applied.

K. Background. A single constant background value is input for each pollutant.

4. Input and Output: Point and area source data, as well as meteorological data must be input to the model. Output from the model includes: input data; one month to one year averaging time simulated (arithmetic mean only); arbitrary averaging time by the Larsen (1969) procedure (typically 1-24 hours) which assumes a lognormal concentration distribution and a power law dependence of median and maximum concentrations on the averaging time; an arbitrary number and location of receptors; an individual point and area source culpability list for each receptor; and a point and area concentration rose for each receptor.

5. System Resource Requirements: The models are written in FORTRAN V. The programs do not require any special software or utilities. Both models require approximately 22K words of core storage for execution on the Univac 1110.


CDMQC, CDM
Block Data
Clint
Calq
Area
Point
end

FLOWCHART FOR CDMQC AND CDM

6. Applications: The source programs for these dispersion models is available as part of UNAMAP (Version 3), PB. 227-193 for $420 from Computer Products, NTIS, Springfield, VA 22161.

7. Technical Contact

D. Bruce Turner
U.S. Environmental Protection Agency
Environmental Applications Branch
Mail Drop 80
Research Triangle Park
N.C. 27711
FTS 629-4564 COM 919/541-4564

8. References

Busse, A.D. and Zimmerman, J.R., User's Guide for the Climatological Dispersion Model, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, Environmental Monitoring Series, EAP-R4-73-024, 131 p. (NTIS accession number PB 227-346/AS, $4.75 paper copy), 1973.

Brubaker, K.L., Brown, P., and Cirillo, R.R., Addendum to User's Guide for Climatological Dispersion Models, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, EPA-450/3-77-015, 134p. (NTIS accession number PB-274-040, $7.25 paper copy), 1977.

GAUSSIAN PLUME DISPERSION ALGORITHM (VALLEY)

1. Model Overview: VALLEY is a steady-state, univariate Gaussian Plume dispersion algorithm designed for estimating either 24-hour or annual concentrations resulting from emissions from up to 50 (total) point and area sources. Calculations of ground-level pollutant concentrations are made for each frequency designed in an array defined by six stabilities, 16 wind directions, and six speeds for 112 program-designed receptor sites on a radial grid of variable scale. Empirical dispersion coefficients are used and include adjustments for plume rise and limited mixing. Plume height is adjusted according to terrain elevations and stability classes.

2. Functional Capabilities: This dispersion model is capable of estimating concentrations resulting from emissions from up to 50 point and area sources for a time frame of either 24 hours or on an annual basis. The model performs calculations of ground-level pollutant concentrations in an array defined by six stabilities, 16 wind directions, and six wind speeds for 112 program-designed receptor sites on a radial grid of variable scale. The model accounts for plume rise and limited mixing.

3. Basic Assumptions:

A. Source-Receptor Relationship. Each point source is assigned an arbitrary location. Each area source is given an arbitrary location and size. The model provides 112 receptors on a radial grid for 16 directions; relative radial distances are internally fixed, and the overall scale may be modified by the user. The location of the grid center is defined by the user. A unique release height for each point and area source is given by VALLEY. Receptors are at ground level, and ground level elevations above mean sea level are defined by the user. The total number of sources for the model is less than or equal to 50.

B. Emission Rate. A single rate is utilized by each point and area source. Each source is treated by an effective point source approximation, and no temporal variation is allowed.

C. Chemical Composition. This is not applicable to VALLEY.

D. Plume Behavior. The model uses Briggs (1971, 1972) plume rise formula for both point and area sources. Alternately, a single constant plume rise value may be input for any or all sources. VALLEY does not treat fumigation or downwash. If the plume height exceeds the mixing height: 1) for long-term calculations, the ground level concentrations are assumed to be equal to zero, 2) for short-term calculations, the maximum plume height is limited to the mixing height.

E. Horizontal Wind Field. For long-term calculations, the model utilizes the following: climatological approach, 16 wind directions, 6 wind speed classes, no variation in wind speed with height, constant uniform (steady-state) wind assumed, and the user must specify the wind speeds representative of each class (these are not internally defined). For short-term calculations, specifically to predict the second highest 24-hour concentration expected in one year, a Class F stability and a 2.5 m/sec. wind speed with user-defined direction are assumed. These conditions are assumed to exist for 25% of the 24-hour period, and an internal adjustment is made for this. In stable conditions, in complex terrain, concentrations for receptors located above the point of impingement are obtained by linear interpolation between the value obtained at the point of impingement and a value of zero at a height of 400 meters above that point. The value at the point of impingment is taken to be equal to the value 10 meters below the plume centerline. For receptors located below the point of impingement, the effective plume height is equal to the height of the plume above the receptor elevation or 10 meters, whichever is larger. The plume is assumed to remain at a constant elevation following the initial rise. In neutral or unstable conditions, in complex terrain, the plume is assumed to remain at a constant height above the topography, following the initial rise. The model assumes that there is no variation of wind speed with height, and that there is a constant, uniform (steady-state) wind.

F. Vertical Wind Speed. In stable conditions, this is assumed to be equal to zero. In neutral and unstable conditions, the vertical wind speed is assumed such that the plume remains at a fixed height above the terrain.

G. Horizontal Dispersion. VALLEY uses a climatological approach, with sector averaging (narrow plume approximation) for calculating the center values of each of the 16 sectors. The model uses linear interpolation between centerlines, as does the Air Quality Display Model (AQDM). Averaging time for VALLEY is one month to one year for long-term calculations.

H. Vertical Dispersion. The model uses a semi-empirical/ Gaussian plume. In the urban mode, the model assumes the following: five stability classes (Turner, 1964); neutral stability split internally into 60% day and 40% night; dispersion coefficients from Pasquill (1961) and Gifford (1961); neutral dispersion coefficients used for all neutral and stable classes; no provision for variations in surface roughness; and stable cases are never dealt with. In the rural mode, the model assumes: six stability classes (Turner, 1964); dispersion coefficients from Pasquill (1961) and Gifford (1961); neutral stability split internally into 60% day and 40% night (has no effect on dispersion coefficients); long term mode only; and no adjustments are made for variation in surface roughness.

I. Chemistry/Reaction Mechanism. VALLEY uses exponential decay and a user-input half-life.

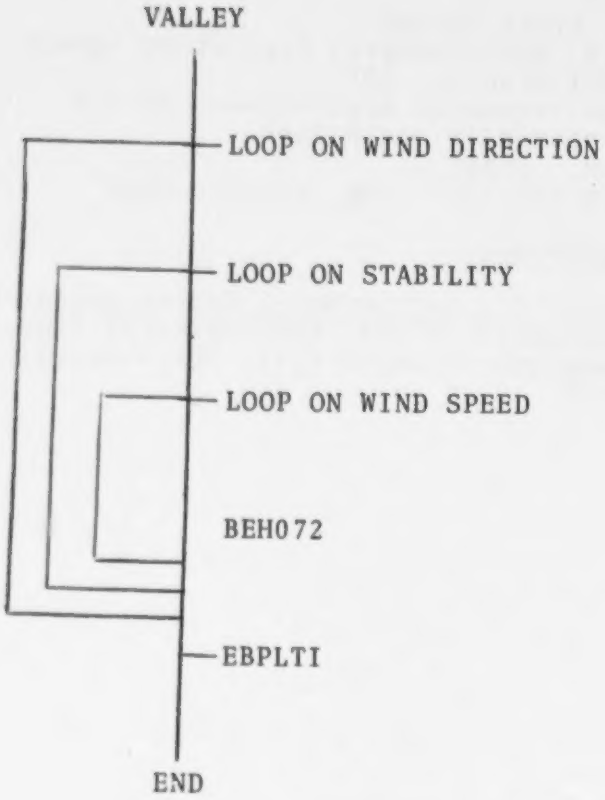
J. Physical Removal. The model uses exponential decay and a user-input half-life.

K. Background. VALLEY does not treat this in any mode.

4. Input and Output: Input to the model includes: point and area residual discharges and stack parameters; meteorological data; and ambient air concentration measurements. Output from the model in the long-term mode includes long-term arithmetic means and a source contribution list for each receptor. Output for the short-term mode includes the second highest 24-hour concentration and a source contribution list for each receptor.

5. System Resource Requirements: VALLEY is written in FORTRAN V. The program does not require any special software or utilities. Approximately 13K words of core memory are required to execute on the Univac 1110.

6. Applications: The source program for this dispersion model is available as part of UNAMAP (Version 3), PB 277 193 for $420 from Computer Products, NTIS, Springfield, VA 22161.


VALLEY
LOOP ON WIND DIRECTION
LOOP ON STABILITY
LOOP ON WIND SPEED
BEH072
EBPLTI
END

VALLEY FLOWCHART

7. Technical Contact

D. Bruce Turner
U.S. Environmental Protection Agency
Mail Drop 80, EPA
Environmental Applications Branch
Research Triangle Park
N.C. 27711
FTS 629-4564 COM 919/541-4564

8. References

Burt, E., Valley Model User's Guide, Publication No. EPA-450/2-77-018, Environmental Protection Agency, Research Triangle Park, North Carolina 27711, September 1977.

GAUSSIAN PLUME MULTIPLE SOURCE AIR QUALITY ALGORITHM (RAM)

1. Model Overview: This short-term Gaussian steady-state algorithm estimates concentrations of stable pollutants from urban point and area sources. Hourly meteorological data are used, and hourly concentrations and averages over a number of hours can be estimated. The Briggs plume rise and the Pasquill-Gifford dispersion equations with dispersion parameters thought to be valid for urban areas are used in the model. Concentrations from area sources are determined using the method of Hanna, that is, sources directly upwind are considered representative of area source emissions affecting the receptor. Special features include determination of receptor locations downwind of significant sources and determination of locations of uniformly spaced receptors to ensure good area coverage with a minimum number of receptors.

2. Functional Capabilities: Concentrations are estimated hourly and for a longer averaging time (less than 24 hours) for a limit of 150 receptor locations (all at the same height above ground) from no more that 250 point sources and 100 area sources.

3. Basic Assumptions:

A. Source-Receptor Relationship. The model assumes an arbitary location for point sources, and the receptors may be: 1) arbitrarily located, 2) internally located near individual source maxima, or 3) on a program-generated hexagonal grid to give good coverage to a user-specified portion of the region of interest. Receptors are all assumed to be at the same height above (or at) ground, and a flat terrain assumed. The model uses a unique stack height for each point source. The model user may specify up to three effective release heights for area sources, each assumed appropriate for a 5 m/sec wind speed. The value used for any given area source must be one of these three. A unique separation for each source-receptor pair is used.

B. Emission Rate. The model assumes a unique constant emission rate for each point and area source. Area source treatment encompasses: narrow plume approximation; area source used as input (not subdivided into uniform elements); arbitrary emission heights input by user; areas must be squares (side length = integer multiples of a basic unit); effective emission height equals that appropriate for a 5 m/sec wind; and the area source contributions are obtained by numerical integration along upwind distance of narrow-plume approximation formulae for contribution from area sources with given effective release heights.

C. Chemical Composition. This is treated as a single inert pollutant.

D. Plume Behavior. The model uses Briggs[8,9,10] plume rise formulas and does not treat fumigations or downwash. If the plume height exceeds the mixing height, the ground level concentration is assumed to be zero.

E. Horizontal Wind Field. The model uses user-supplied hourly wind speeds and user-supplied hourly wind directions (nearest 10°), internally modified by addition of a random integer value between -4° and +5°. Wind speeds are corrected for release height based on power law variation, exponents from DeMarrais[6]; different exponents for different stability classes are used, and the reference height is equal to 10 meters. A constant, uniform (steady-state) wind is assumed within each hour.

F. Vertical Wind Speed. This is assumed to be equal to zero.

G. Horizontal Dispersion. The model uses a semi-empirical/ Gaussian plume. Hourly stability class is determined internally by Turner[3] procedure (six classes are used). Dispersion coefficients are from McElroy and Pooler[4] (urban) or Turner[3] (rural). No further adjustments are made for variations in surface roughness or transport time.

H. Vertical Dispersion. A semi-empirical/Gaussian plume is used. Hourly stability class is determined internally. Dispersion coefficients are from McElroy and Pooler[4] (urban) or Turner[7] (rural). No further adjustments are made for variations in surface roughness.

I. Chemistry/Reaction Mechanism. The model assumes an exponential decay with a user-input half-life.

J. Physical Removal. Exponential decay and a user-input half-life are used.

K. Background. This is not treated.

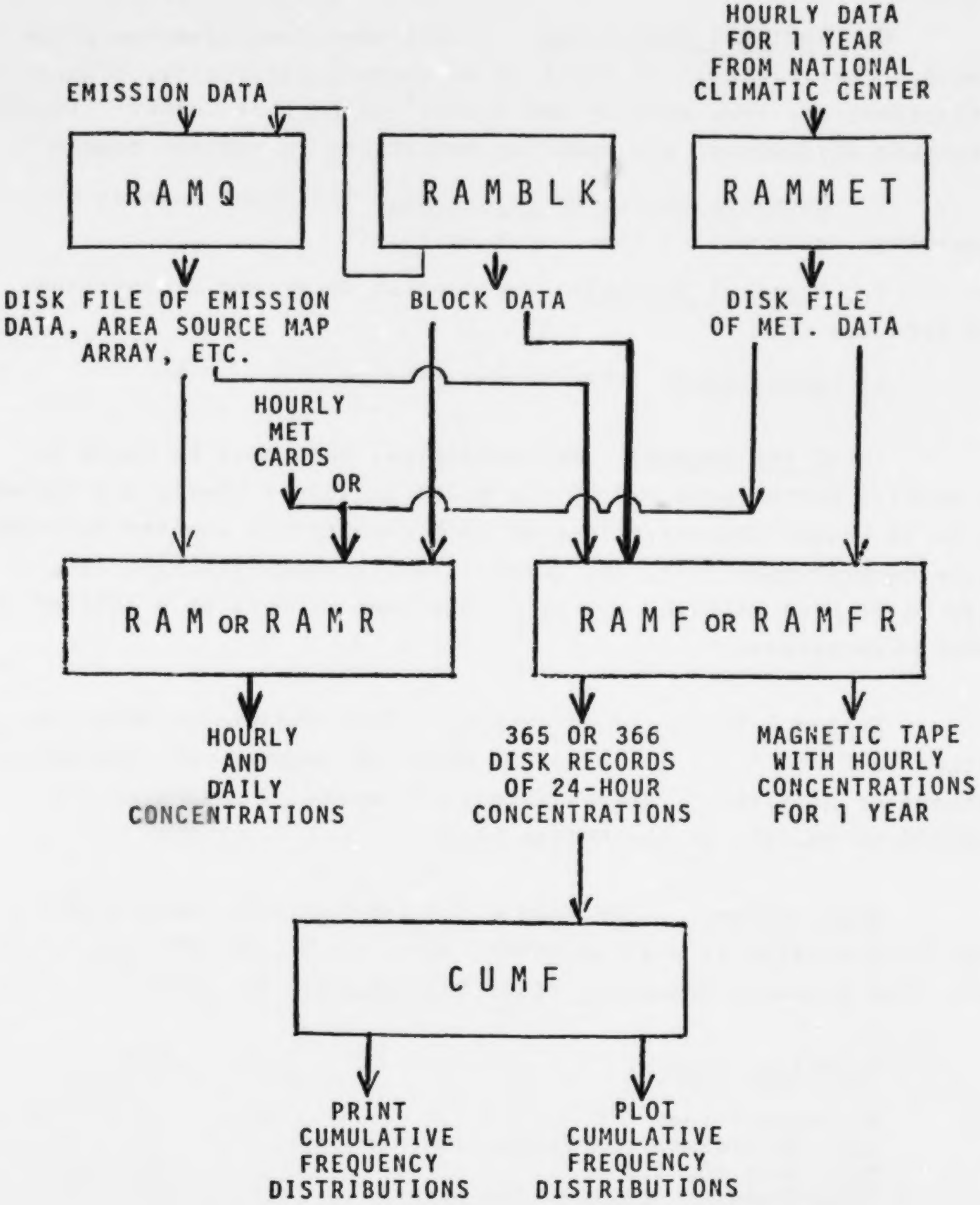
4. Input and Output: Meteorological data must be input to the model. Output produced by the model includes: hourly and average (up to 24 hours) concentrations at each receptor; a limited individual source contribution list; and cumulative frequency distribution based on 24-hour averages and up to one year of data at a limited number of receptors.

5. System Resource Requirements: This dispersion model is written in FORTRAN V. The program does not require any special software or utilities. Approximately 41K words of core are required to execute on the Univac 1110.

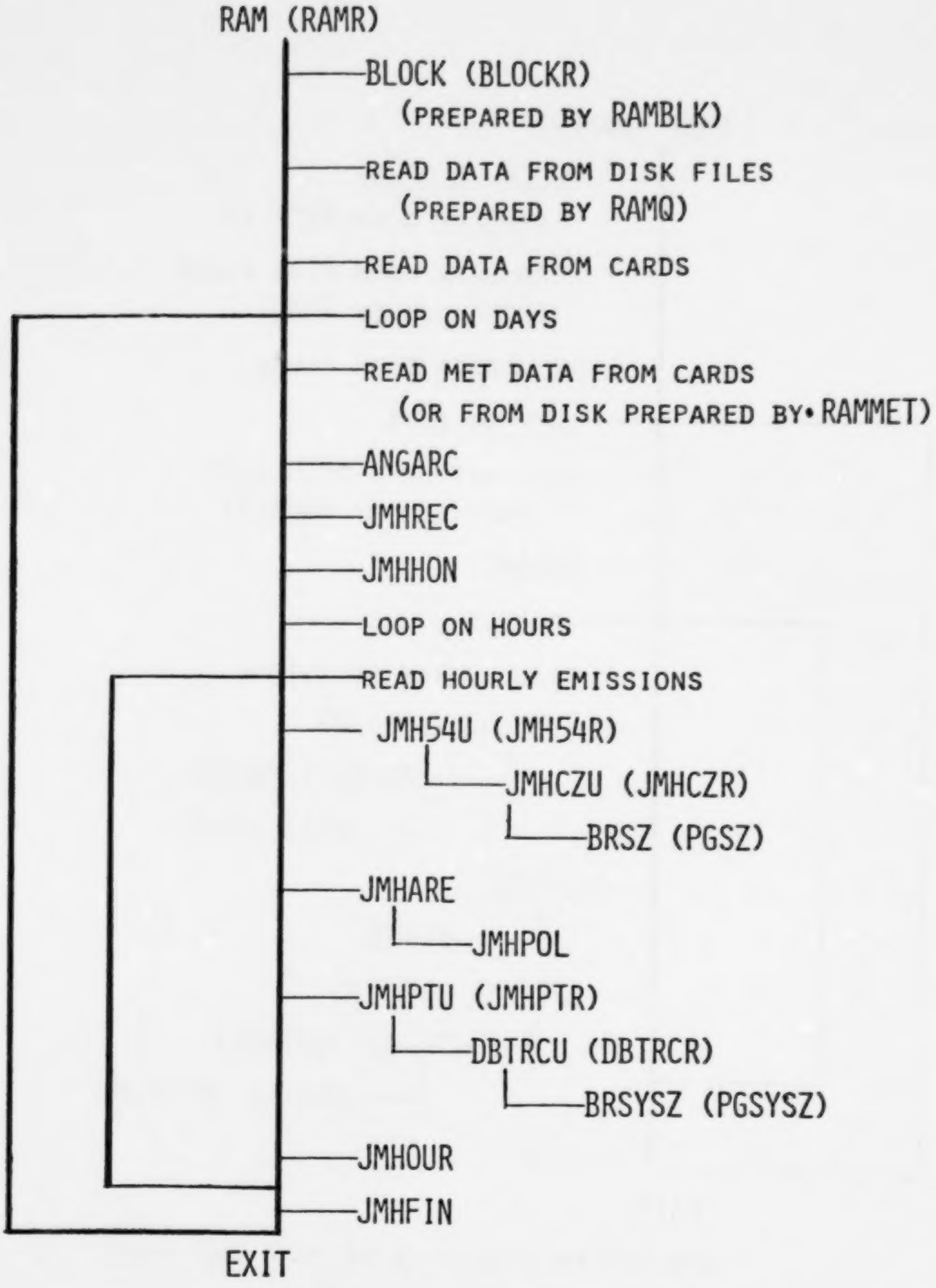
6. Applications: The source program for this dispersion model is available as part of UNAMAP (Version 3), PB 277 193, $420, from Computer Products, NTIS, Springfield, VA 22161.

7. Technical Contact

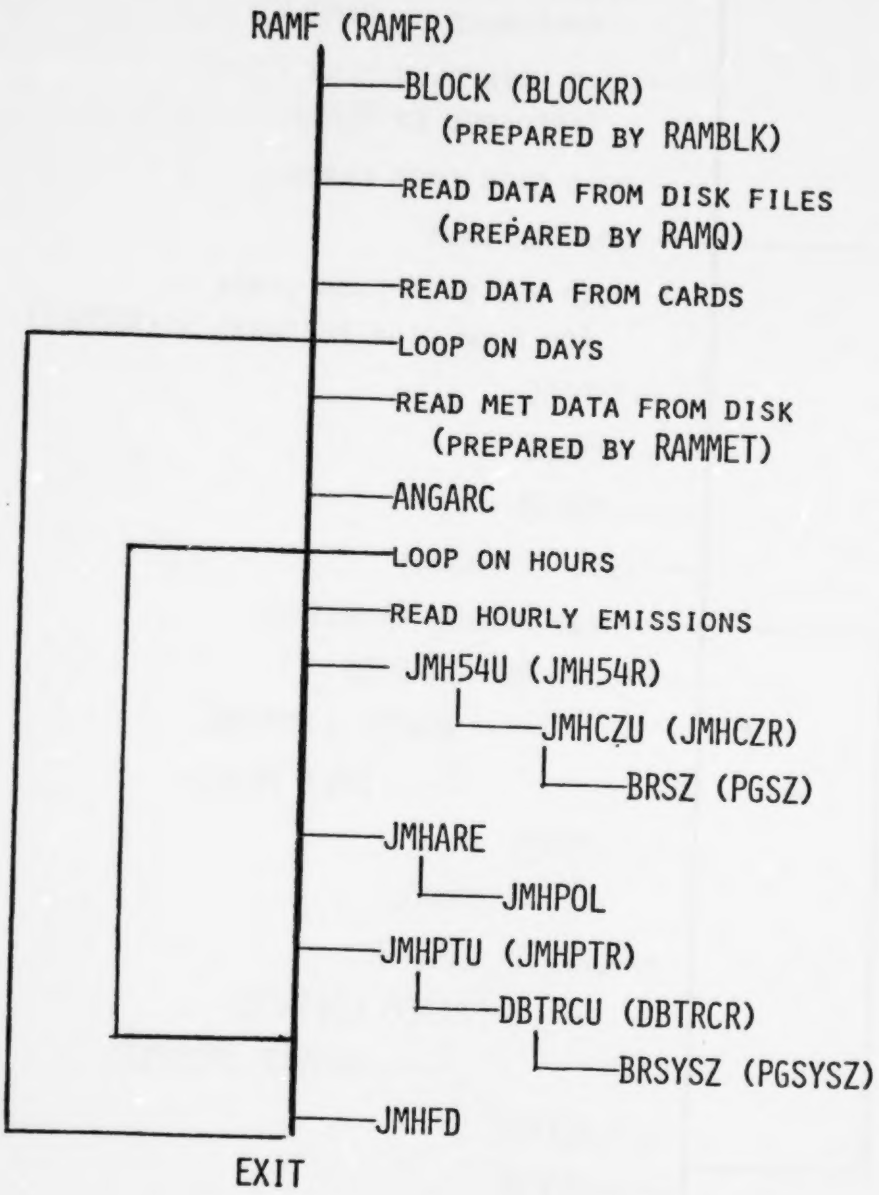
D. Bruce Turner
U.S. Environmental Protection Agency
Mail Drop 80, EPA
Environmental Applications Branch
Research Triangle Park
N.C. 27711
FTS 629-4564 COM 919/541-4564


HOURLY DATA FOR 1 YEAR FROM NATIONAL CLIMATIC CENTER
EMISSION DATA
RAMQ
RAMBLK
RAMMET
DISK FILE OF EMISSION DATA, AREA SOURCE MAP ARRAY, ETC.
BLOCK DATA
DISK FILE OF MET. DATA
HOURLY MET CARDS
OR
RAM OR RAMR
RAMF OR RAMFR
HOURLY AND DAILY CONCENTRATIONS
365 OR 366 DISK RECORDS OF 24-HOUR CONCENTRATIONS
MAGNETIC TAPE WITH HOURLY CONCENTRATIONS FOR 1 YEAR
CUMF
PRINT CUMULATIVE FREQUENCY DISTRIBUTIONS
PLOT CUMULATIVE FREQUENCY DISTRIBUTIONS

Interrelationships of RAM System Main Programs


RAM (RAMR)
BLOCK (BLOCKR)
(PREPARED BY RAMBLK)
READ DATA FROM DISK FILES
(PREPARED BY RAMQ)
READ DATA FROM CARDS
LOOP ON DAYS
READ MET DATA FROM CARDS
(OR FROM DISK PREPARED BY RAMMET)
ANGARC
JMHREC
JMHHON
LOOP ON HOURS
READ HOURLY EMISSIONS
JMH54U (JMH54R)
JMHCZU (JMHCZR)
BRSZ (PGSZ)
JMHARE
JMHPOL
JMHPTU (JMHPTR)
DBTRCU (DBTRCR)
BRSYSZ (PGSYSZ)
JMHOUR
JMHFIN
EXIT

Subroutine Structure of RAM and RAMR


RAMF (RAMFR)
BLOCK (BLOCKR)
(PREPARED BY RAMBLK)
READ DATA FROM DISK FILES
(PREPARED BY RAMQ)
READ DATA FROM CARDS
LOOP ON DAYS
READ MET DATA FROM DISK
(PREPARED BY RAMMET)
ANGARC
LOOP ON HOURS
READ HOURLY EMISSIONS
JMH54U (JMH54R)
JMHCZU (JMHCZR)
BRSZ (PGSZ)
JMHARE
JMHPOL
JMHPTU (JMHPTR)
DBTRCU (DBTRCR)
BRSYSZ (PGSYSZ)
JMHFD
EXIT

Subroutine Structure of RAMF and RAMFR

8. References

Novak, J.H. and Turner, D.B., "An Efficient Gaussian Plume Multiple-Source Air Quality Algorithm," Journal of the Air Pollution Control Association, 26 (6), 560-575, 1976.

HIWAY MODEL (HIWAY)

1. Model Overview: HIWAY is an interactive program which computes the hourly concentrations of non-reactive pollutants downwind of roadways. It is applicable for uniform wind conditions and level terrain. Although best suited for at-grade highways, it can also be applied to depressed highways (cut sections). The "User's Guide for HIWAY: A Highway Air Pollution Model," is available for EPA as EPA-650/4-74-008 and from NTIS (accession number PB 239-944/AS).

2. Functional Capabilities: Hourly estimates of concentrations for receptors off roadways are determined resulting from a single at-grade or cut-section roadway segment. The user specifies geometry and emissions of roadway segment, meteorological conditions to be simulated, and receptor coordinates and height of receptor above ground.

3. Basic Assumptions:

A. Source-Receptor Relationship: The model uses a horizontal finite line with multiple line sources (up to 24 lines). These are straight lines, arbitrary in orientation and length. One road or highway segment is run at a time. Receptors are arbitrarily located, downwind of the sources, with a unique source-receptor distance defined. Arbitrary receptor heights and arbitrary release heights are used. In the cut section mode receptors cannot be located in the cut, and emissions are treated as coming from 10 equal uniform line sources at the top of the cut. A flat terrain is assumed, and line sources are treated as a sequence of point sources; the number is such that convergence to within 2% is achieved.

B. Emission Rate: A constant uniform emission rate for each lane is assumed.

C. Chemical Composition: This is not applicable to the model.

D. Plume Behavior: This is not treated.

E. Horizontal Wind Field. The user specifies arbitrary wind speed and direction. No variation of wind speed and direction with height is allowed, and a uniform, constant (steady-state) wind is assumed.

F. Vertical Wind Speed. This is assumed to be equal to zero.

G. Horizontal Dispersion. The model uses a semi-empirical/ Gaussian plume, and the user specifies which of 6 stability classes to be used: Turner (1964). Dispersion coefficients used are from Turner (1969); for distances less than 100m, dispersion coefficients from Zimmerman and Thompson (1975) are used. In the level grade mode, the initial value of the dispersion coefficient is 3 meters. In the cut section mode, the initial value of the dispersion coefficient is approximated as a function of the wind speed. No further adjustments to the dispersion coefficients are made.

H. Vertical Dispersion. The model uses a semi-empirical/ Gaussian plume in which the user specifies stability class. Dispersion coefficients used are from Turner (1969); for distances less than 100m, dispersion coefficients from Zimmerman and Thompson (1975) are used. In the level grade mode, the initial σ_z is equal to 1.5 meters. In the cut section mode, the initial σ_z is equal to a function of the wind speed.

I. Chemistry/Reaction Mechanism. This is not treated.

J. Physical Removal. This is not treated.

K. Background. This is not treated.

4. Input and Output: Initial set-up and calibration needs are: (1) in batch mode residual discharges for vehicular line sources are input and in interactive mode residual discharges are either

input or they may be requested from program; (2) meteorological data: wind speed, wind direction, stability class, mixing height; (3) ambient air concentration measurements. For verification of the model, meteorological date and ambient air concentrations are needed. Output from the model includes a printout of the 1-hour average concentration at each receptor.

5. System Resource Requirements: This dispersion model is written in FORTRAN V. The program does not require any special software or utiliities. Approximately 12K words of core are required to execute on the Univac 1110.

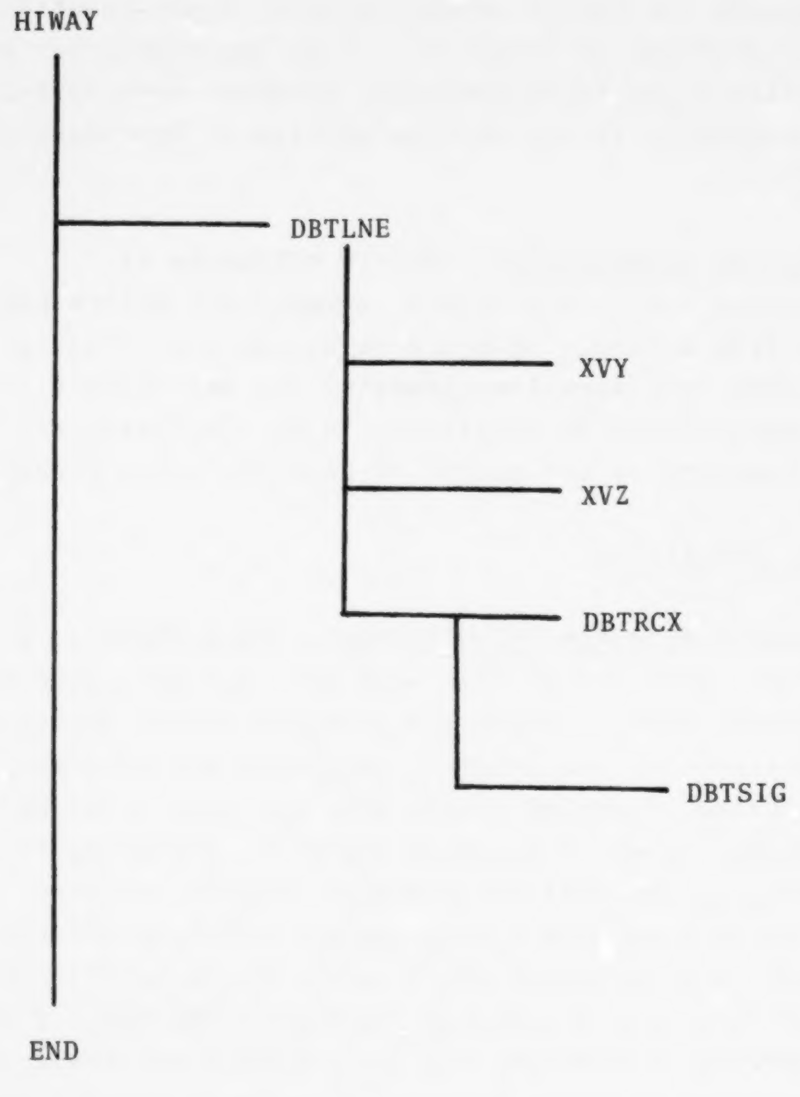
6. Applications: The source program for this dispersion model is available as part of UNAMAP (Version 3), PB 277 193 for $420 from Computer Products, NTIS, Springfield, VA 22161.

7. Technical Contact

D. Bruce Turner
U.S. Environmental Protection Agency
Mail Drop 80
Environmental Applications Branch
Research Triangle Park, NC 27711
FTS 629-4564 COM 919/541-4564

8. References:

Zimmerman, J.R., and Thompson, R.S., 1975: User's Guide for HIWAY: A Highway Air Pollution Model. U.S. Environmental Protection Agency, Research Triangle Park, NC. Environmental Monitoring Series, EPA-650/4-74-008, 59 p. (NTIS accession number PB 239-944/AS).


HIWAY
DBTLNE
XVY
XVZ
DBTRCX
DBTSIG
END

FLOWCHART FOR HIWAY

HIWAY-2

1. Model Overview: HIWAY-2 is a batch and interactive program which computes the hourly concentrations of non-reactive pollutants downwind of roadways. It is applicable for uniform wind conditions and level terrain. Although best suited for at-grade highways, it can also be applied to depressed highways (cut sections).

2. Functional Capabilities: Hourly estimates of concentrations for receptors off roadways are determined resulting from a single at-grade or cut-section roadway segment. The user specifies geometry and emissions of roadway segment, meteorological conditions to be simulated, and receptor coordinates and height of receptor above ground.

3. Basic Assumptions:

   A. Source-Receptor Relationship: The model uses a horizontal finite line with multiple line sources (up to 24 lines). These are straight lines, arbitrary in orientation and length. Receptors are arbitrarily located, downwind of the sources, with a unique source-receptor distance defined. Arbitrary receptor heights and arbitrary release heights are used. In the cut-section mode the receptors cannot be located in the cut, and emissions are treated as coming from 10 equal uniform line sources at the top of the cut. A flat terrain is assumed, and line sources are treated as a sequence of point sources; the number is such that convergence to within 2% is achieved.

   B. Emission Rate: A constant uniform emission rate for each lane is assumed.

C. Chemical Composition: This is not applicable to the model.

D. Plume Behavior: This is not treated.

E. Horizontal Wind Field: The user specifies arbitrary wind speed and direction. No variation of wind speed and direction with height is allowed, and a uniform, constant (steady-state) wind is assumed.

F. Vertical Wind Speed: This is assumed to be equal to zero.

G. Horizontal Dispersion: The model uses a semi-empirical/Gaussian plume, and the user specifies which of 6 stability classes are to be used (Turner, 1964). For distances less than 300 m, empirically derived dispersion parameters are used (Rao, et al., 1980). In the level grade mode, the initial value of the dispersion coefficient is twice the value for the initial vertical dispersion coefficient. In the cut-section mode, the initial value of the dispersion coefficient is approximated as a function of the wind speed.

H. Vertical Dispersion: The model uses a semi-empirical/Gaussian plume in which the user specifies stability class. The dispersion coefficients used are from Turner (1969); for distances less than 300 m dispersion coefficients (Rao, et al., 1980) are used. In the level grade mode, the initial σ_z is a function of the crosswind component with a maximum value of 3.57 m and a minimum value of 1.5 m. In the cut-section mode the initial dispersion parameter is a function of wind speed.

I. Chemistry/Reaction Mechanism. This is not treated.

J. Physical Removal. This is not treated.

K. Background. This is not treated.

4. Input and Output: Initial set-up and calibration needs are: (1) in both batch and interactive mode, discharges for vehicular line sources are input into the program; (2) meteorological data: wind speed, wind direction, stability class, mixing height; and (3) ambient air concentration measurements. For verification of the model, meteorological data and ambient air concentrations are needed.

Output from the model includes a printout of the one-hour average concentration at each receptor.

5. System Resource Requirements: HIWAY-2 is written in FORTRAN and is run on the Univac 1110. It requires 6K bytes of core storage for execution. An operator with knowledge in engineering will be useful.

6. Applications: The source program for this dispersion model is available as a part of UNAMAP (Version 3), PB 277-193 for $420 from Computer Products, NTIS, Springfield, VA 22161.

7. Technical Contact

William B. Petersen
U.S. Environmental Protection Agency
Environmental Science Research Laboratory
Research Triangle Park
N.C. 27711
COM 919/541-4564 FTS 629-4564

8. References

Petersen, W.B., 1980. User's Guide for HIWAY-2: A Highway Air Pollution Model. U.S. Environmental Protection Agency, Research Triangle Park, N.C., EPA-600/8-80-018, 70 p. (Also available from NTIS as PB 80-227-576).

Rao, S.T. and Keenan, M.T., 1980: Suggestions for Improvement of the EPA-HIWAY Model. JAPCA, 30, 6, pp. 247-256.

INDUSTRIAL SOURCE COMPLEX MODEL (ISC)

1. Model Overview: The Industrial Source Complex Dispersion Model is a Gaussian plume model used to evaluate the air quality impact of emissions from industrial source complexes. The ISC Model consists of two computer programs, one for short-term analyses and one for long-term analyses. The short-term model program, ISCST, uses sequential hourly meteorological data to estimate the concentration or deposition patterns from one hour to one year. The long-term model program, ISCLT, uses statistical wind summaries to estimate the seasonal and annual concentration or deposition patterns. The ISC Model has rural and urban options. Major features of the ISC Model program are: (1) the effects of aerodynamic building wakes and stack tip downwash; (2) the effects of variations in terrain height; (3) the plume rise due to momentum and bouyancy as a function of downwind distance; (4) the dispersion of emissions from stack area, line, and volume sources where line sources are simulated by multiple volume sources; (5) the physical separation of multiple sources; (6) the time-dependent exponential decay of pollutants; and (7) the effects of gravitational settling and dry deposition.

2. Functional Capabilities: The number of sources and receptors are interdependent. However, 300 is the maximum number of sources accepted, arbitrarily located. Receptors can be specified on a polar or rectangular grid and Briggs` early plume rise formulations, including the momentum terms, are used. Deposition can be calculated or allowed for over flat terrain only. The short-term program calculates values of average concentration or deposition for time periods of 1, 2, 3, 4, 6, 8, 12, and 24 hours. Additionally, the ISCST may be

used to calculate N-day concentration or deposition values where the maximum value of N is 366 days. The units option allows the user to specify the input emissions units and/or output concentration or deposition units. Applications that do not require at least one of the ISC Model features should utilize a less comprehensive computer model.

3. Basic Assumptions: Meteorological homogeneity is assumed following the conversion of surface wind speed to that at plume height. All plumes remain level, regardless of terrain elevation, unless significant terminal fall velocity is specified. Emission rates can be varied according to specified meteorological classes or as a function of time (hour of day, season or month, or both). A simple time dependent exponential decay of the pollutant is optional.

4. Input and Output: The input of the meteorological data required for ISCST are mean wind speed and measurement height, average random flow vector, wind profile exponents*, ambient air temperature, height of mixing layer, Pasquill stability, and vertical potential temperature gradient*. These data may be input directly using the same preprocessed meteorological data tape as the CRSTER Model or alternatively input by card deck. For ISCLT, joint frequencies of occurrence of wind speed, direction, and stability are required. Source data consists of emission rate (total emissions for deposition); dimensions of stack, building area, or volume source; effluent characteristics; surface reflection coefficients for each settling-velocity category; receptor data; and receptor terrain elevation data.

*Default values are available.

Output can be directed to a line printer and/or magnetic tape. Five categories of printed output can be acquired from ISCST: input source-receptor and hourly meteorological data listings; concentration or deposition values calculated for any combination of sources at all receptors for any specified day(s) or time period; highest and second-highest such values; and a maximum of 50 such values. ISCLT output provides input source-receptor and meteorological data listings; long-term mean concentration or deposition values calculated at each receptor for each source and for combined emission sources; and contributions of individual sources to the maximum 10 such values calculated for the combined emission sources or as contributed to user specified receptors.

5. System Resource Requirements: The ISC Model programs are written in FORTRAN IV and require approximately 65,000 Univac 1110 words. The programs may also be used on a medium to large IBM or CDC computer system with little or no modification.

6. Applications: The ISC Model is recommended for use in air quality assessments of stack, area, and volume industrial complex sources in urban and rural areas where short-term, seasonal, and/or annual air quality concentration estimates of stable pollutants are required.

7. Technical Contact

Joseph A. Tikvart
U.S. Environmental Protection Agency
Office of Air Quality Pollution Standards
Mail Drop 14
Research Triangle Park
N.C. 27711
COM 919/541-5251 FTS 629-5251

8. Reference

Industrial Source Complex (ISC) Dispersion Model User's Guide, Volume I; NTIS # PB 80-133044.

Industrial Source Complex (ISC) Dispersion Model User's Guide, Volume II (Appendices A through I) NTIS # PB 80-133051.

Magnetic Tape of Programs NTIS # PB 80-133036.

KINETIC MODEL AND OZONE ISOPLETH PLOTTING PACKAGE (OZIPP)

1. Model Overview: The Kinetics Model and Ozone Isopleth Plotting Package (OZIPP) computer program can be used to simulate ozone formation in urban atmospheres. OZIPP calculates the maximum one-hour average ozone concentrations given a set of input assumptions about initial precursor concentrations, light intensity, dilution, diurnal and spatial emission patterns, transported pollutant concentrations, and reactivity of the precursor mix. The results of multiple simulations are used to produce an ozone isopleth diagram tailored to particular cities. Such a diagram relates maximum ozone concentrations to concentrations of non-methane organic compounds and oxides of nitrogen, and can be used in the Empirical Kinetic Modeling Approach (EKMA) to calculate emission reductions necessary to achieve air quality standards for photochemical oxidants.

2. Functional Capabilities: The major function of the OZIPP Model is to generate an ozone isopleth diagram representative of a particular city. The diagram explicitly depicts the maximum, one-hour average concentrations of ozone occuring within or downwind of a city as a function of precursor levels existing within the city in the early morning. These diagrams are based on mathematical simulations of ozone formation occurring during a day. As such, the model is limited in applicability to ozone problems within or immediately downwind of urban areas and cannot consider the following: rural ozone problems; ozone problems occurring in the early morning or at night; and contributions of single or small groups of sources to ozone problems. The OZIPP model is best used to study the effectiveness of areawide control strategies in reducing peak, one-hour average ozone concentrations within or downwind of a city.

3. Basic Assumption: The model underlying OZIPP is similar in concept to a trajectory-type photochemical model which simulates the formation of ozone from precursors within a migrating column of air. A column of uniformly mixed air extends from the earth's surface throughout the mixed layer. The height of the column rises according to the diurnal variation in mixing height, resulting in dilution of pollutants within the column and entrainment of pollutants which were initially above the column. As the column moves, emissions of fresh precursors are encountered. The model mathematically calculates the formation of ozone within the column as a function of time in accordance with a chemical kinetic mechanism. The model employs a gear-type integration scheme to numerically solve the set of differential evaluations which describe the model assumptions.

To generate an ozone isopleth diagram, the model performs repeated simulations with differing pollutant levels initially within the column. Using the results of these simulations, a diagram is constructed which expresses the calculated peak and one-hour average ozone concentrations as a function of the initial precursor concentrations. The program incorporates a hyperbolic spline interpolation scheme to construct the graph.

4. Input and Output: Data are supplied to the model to make an ozone isopleth diagram specific to a particular city. These data include: latitude, longitude and time zone of the city; the day, month and year; the minimum morning and maximum afternoon mixing heights; sets of emission fractions which reflect the effect of precursor emissions occuring throughout the day; and the concentration of ozone and precursor transported into the city. Additional input parameters are supplied to control the generation of the ozone isopleth

diagram (e.g., scales of the diagram, size of the diagram, accuracy, interpolation smoothing, etc.). All input data are processed in a simple manner, and no extensive computerized data base is required.

The primary output of the model is the ozone isopleth diagram. The diagram is depicted on a line printer plot, and can be generated as an option on a Calcomp Plotter. A report is also produced which summarizes the input data and results of the simulations that were performed to generate the diagram. Operation includes training in computer programming and engineering.

5. System Resource Requirements: OZIPP is coded in FORTRAN. It can be run on a Univac 1100 mainframe with a 132 position line printer and a card reader/punch. A Calcomp plotter may be used as an option. Operator requirements include training in computer programming and engineering.

6. Applications: The OZIPP Model has been used to generate ozone isopleth diagrams to calculate emission reductions necessary to achieve the ambient air quality standard for ozone. The model was used by state/local air pollution control agencies as the basis for estimating emission reductions for the 1979 submittal of the State Implementation Plans.

7. Technical Contact

Gerald L. Gipson
U.S. Environmental Protection Agency
OAQPS/MDAD/AMTB/TDS
Mail Drop 14
Research Triangle Park
N.C. 27711
COM (919) 541-5522 FTS 629-5522

8. References

Kinetics Model and Ozone Isopleth Plotting Package (OZIPP), EPA-600/8/770014b, U.S. Environmental Protection Agency, Research Triangle Park, N.C., July 1978.

Whitten, G.Z. and Hugo, H. User's Manual for Kinetics Model and Ozone Isopleth Plotting Package, EPA-600/8-78-014a, U.S. Environmental Protection Agency, Research Triangle Park, N.C., July 1978.

Users, Limitation and Technical Basis of Procedures for Quantifying Relationships Between Photochemical Oxidants and Precursors, EPA-450/2-77-021a, U.S. Environmental Protection Agency, Research Triangle Park, N.C., November 1977.

LAGRANGIAN PHOTOCHEMICAL AIR QUALITY SIMULATION MODEL (LPAQSM)

1. Model Overview: LPAQSM is designed to predict the concentrations of ozone produced in an urban area by modeling the emissions, transport, and transformations in the presence of ultraviolet radiation.

2. Functional Capabilities: The model is designed for simulation between sunrise and sunset on a single day. It has five levels of vertical resolution but describes only one area of an urban domain at a particular time. Concentrations are output for each 30 minutes along the trajectory.

3. Basic Assumptions: The model assumes a Lagrangian parcel of air of dimensions typically 5x5 km by 1.5 km high. The parcel moves with the wind, entraining emissions which enter into the photochemical reactions. The initial leading of pollutants is specified and the parcel has a rigid upper boundary and no lateral diffusion.

4. Input and Output: Input for this model includes the following data:

    1. Emissions inventory for hydrocarbons and nitrogen oxide.
    2. Surface network air quality and meteorological measurements.
    3. Upper air radiosonde data.
    4. Solar radiation data.

The Regional Air Pollution Study (RAPS-St. Louis) data base is being used with LPAQSM.

Output is in the form of a computer printout. Concentrations of ozone, carbon monoxide, sulfur dioxide, hydrocarbons, and nitrogen oxides are supplied at 30 minute intervals for 5 levels in the vertical.

5. System Resource Requirements: LPAQSM is coded in FORTRAN and is run on an Univac 1110 mainframe. The model requires 60,000 words of core storage for execution. It is stored on 2 magnetic tapes and requires a line printer for output. Operating skills for the model include a programmer.

6. Applications: The model builder, Environmental Research and Technology, Inc., has tested the model against data in Los Angeles as well as using it in environmental impact assessments.

7. Technical Contact

Jack Shreffler
U.S. Environmental Protection Agency
Environmenal Sciences Research Laboratory
Research Triangle Park
N.C. 27711
COM 919/541-4524 FTS 629-4524

8. References

A Lagrangian Photochemical Air Quality, Simulation Model
Vol. I. Model Formulation Vol. II. User's Manual
EPA-600/8-79-015a,b.

LIVERMORE REGIONAL AIR QUALITY MODEL (LIRAQ)

1. Model Overview: The Livermore Regional Air Quality Model (LIRAQ) exists in two versions, LIRAQ-1 and LIRAQ-2. Both versions are two-dimensional (horizontal) Eulerian grid models designed to predict regional distributions of air pollutants. LIRAQ-1 can treat up to four noninteracting or simply interacting species on up to a 45 x 50 grid. It uses the flux-corrected algorithm to treat transport. LIRAQ-2 simulates evolution of the concentrations of 12 chemically interacting species on a 20 x 20 grid. It uses an upstream differencing scheme to represent horizontal transport, and the Gear package to carry out time integration. A version with chemistry updated to 1980 is now being tested.

2. Functional Capabilities: Both versions of the model provide graphical and tabular displays of selected species over the entire grid, and graphical displays of the temporal variability of selected species at up to 50 selected grid elements. Edit intervals are as specified and can be varied at the user's convenience. Extensive graphical capabilities are built into the code, and all input quantities are echoed in tabular output. Temporal and spatial variations of emissions, mixing depth, winds, solar flux, K_z, and spatial variations of terrain are treated.

3. Basic Assumptions: Both of the LIRAQ models are 2-D horizontal models bounded on the top by a temporally and spatially varying inversion "lid." Both models assume a logarithmic concentration profile in the vertical based on a balance of fluxes at the boundaries which can be different for each species. This vertical profile is assumed to interact with the power law wind profile in determining horizontal transport. LIRAQ-2 does not compensate for the effects of the vertical distribution of pollutants in calculating transformation by chemical reactions. LIRAQ-2 uses a chemical reaction mechanism of some complexity but uses an approximate "lumping" scheme in treating hydrocarbon emissions and other reactive organic species. Although developed with the intention of maintaining the maximum fidelity to real

chemical data compatible with the model, the chemical mechanism is, in part, a simulation mechanism. The present version of LIRAQ-1 assumes no chemical interactions other than a deposition velocity and/or exponential decay.

4. Input and Output: Inputs for the initial set-up and calibration of the model include:

1) A file specifying the topographic elevation at every grid point in the model domain, as well as any map information (rivers or shore outlines, city or station locations) to be displayed on the output.
2) Files specifying the emissions in each grid element at hourly intervals.
3) Files giving data fields on mass consistent vertical (through the inversion) and horizontal fluxes, inversion base heights (i.e. mixing depths), atmospheric transmissivity (based on cloud extent), and horizontal and vertical eddy diffusivities. These files are normally supplied by a meteorological data processing code, MASCON, but could be provided by other processing routines.
4) A file giving photodissociation rates as a function of solar zenith angle for a clear sky (LIRAQ-2 only).
5) A file giving observed species concentrations at measuring stations to be used for initializing the problem.
6) A file defining the particular problem to be run (i.e. title, start time, stop time, species and locations for graphical output, boundary conditions, molecular weights, and specific emissions factors for various species).

Outputs provided by the model include the following:

1) Voluminous printer files echoing all input and providing species concentrations at the surface and averages for the mixed layer at all grid locations at every edit interval.
2) A file containing concentrations for selected species at selected locations as a function of time.
3) A file containing information about the numerical integration scheme.

4) Voluminous graphical output as described above.

5. System Resource Requirements: The LIRAQ models are coded in FORTRAN IV and require a CDC 7600 or equivalent with random access disks. Typical problems take 0.1-0.3 hours for LIRAQ-1 and 0.5-1.0 hours for LIRAQ-2, thus pointing to the need for adequate resources to fund computer time needs. The program presently exists only at the Lawrence Berkeley and Lawrence Livermore Laboratories. A computer programmer, a research assistant, and an experienced modeler with expertise in coding, diffusion models, and advanced mathematical solution techniques are useful.

6. Applications: Both LIRAQ models have been used by the San Francisco Bay Area Air Pollution Control District and the Association of Bay Area Governments in the preparation of the long-term Air Quality Maintenance Plan for the San Francisco Bay area. The U.S. Environmental Protection Agency has included LIRAQ-2 as part of their model validation exercise gathered during the RAPS program. Processors necessary to make the EPA data base LIRAQ-compatible have been developed. C.D. Craig of Oregon State University is currently involved in a program to use LIRAQ-1 to model the air quality impact of agricultural burning in the Willamette Valley.

7. Technical Contacts

Dr. Jack Shreffler
U.S. Environmental Protection Agency
Environmental Sciences Research Laboratory
Research Triangle Park
N.C. 27711 COM 919/541-3660 FTS 629-3660

M.C. MacCracken, J.J. Walton, and J.E. Penner
Lawrence Livermore Laboratory
Livermore, California 94550
COM 415/422-1800
FTS 422-1800

8. References

ABAG, et al., Application of Photochemical Models: Volume I, The Use of Photochemical Models in Urban Ozone Studies, EPA Report 450/4-79-025, 1979.

Duewer, W.H., et al. "Livermore Regional Air Quality Model (LIRAQ) Transfer to EPA, "Lawrence Livermore Laboratory Report UCRL-52864, 1980 (available from NTIS). Also to be published by EPA.

Duewer, W.H. et al.,"The Livermore Regional Air Quality Model: II., Verification and Sample Application in the San Fransisco Bay Area," J. Appl. Meteorol., 17, 273-311, 1978.

MacCracken, M.C., et al., The Livermore Regional Air Quality Model; Concept and Development," J. Appl. Meteorol., 17, 254-272, 1978.

MacCracken, M.C., et al., User's Guide to the LIRAQ Model; An Air Pollution Model for the San Fransisco Bay Area, Lawrence Livermore Laboratory, Livermore, California, December 1975.

MODIFIED ROLLBACK MODEL (ROLLBACK)

1 Model Overview: The Modified Rollback Model is a computerized air quality simulation model that has been used for assessing the relative air quality impacts of alternative control strategies which are national in scope. Air quality projections for carbon monoxide and nitrogen oxides are made using the Morris-deNevers modified rollback equations. Ozone projections are made using the Empirical Kinetic Modeling Approach (EKMA) standard isopleth diagram. Emission inventory projections are made using data on mobile and stationary source emission factors, VMT growth rates, stationary source retirement rates, growth rates, and control efficiencies.

2. Functional Capabilities: Modified Rollback can be used to estimate changes in CO and annual average NO_2 levels due to assumed changes in CO and NO_x emissions, respectively. Changes in ozone air quality levels are estimated using the standard isopleth diagram of EKMA. These procedures are best used to compare the relative air quality impacts of alternative area source control strategies. The model requires county level, or larger, emissions inventories by major source category.

3. Basic Assumptions: The simple rollback model is based on the assumption that the air quality concentration of a pollutant at a point is equal to the background concentration of that pollutant and some linear function of the total emission rate of that pollutant which influences the concentration at that point. Modified Rollback uses the

Morris-deNevers equations to account for differing rates of growth/reduction in emissions from a number of source categories. The model assumes that the spatial and temporal distributions of emissions and the meteorological conditions remain constant between the base year and the projection year. However, for ozone projections, the model uses the standard EKMA isopleths described in Reference 3.

4. Input and Output: For each study area, the user must furnish data on the base year air quality level; the background concentration; the emissions, growth and retirement rates; and the control efficiencies for each major mobile and stationary source category and strategy scenario. The air quality data is typically obtained from SAROAD and the emissions data from NEDS.

Output reports consist of individual source area emissions inventories for the base year, each projection year/strategy combination, and air quality summary reports. The air quality summary reports, grouped by strategy, display the base year air quality concentration, projection year air quality levels, and expected number of violations of the NAAQS for each study area.

5. System Resource Requirements: ROLLBACK is coded in FORTRAN. It is run on an IBM 360 or Univac 1108 mainframe computer. The model also uses a card reader/punch. It uses a regular line printer for the output. An engineering and computer programming background are useful.

6. Applications: The Modified Rollback Model has been used by EPA to evaluate the relative air quality impacts of revisions to the automotive emission standards. Other applications include the regulatory analyses conducted in association with the review of the ambient air quality standards.

7. Technial Contact

Warren P. Freas
U.S Environmental Protection Agency
Monitoring and Data Anaysis Division
Mail Drop 14
Research Triangle Park
N.C. 27711
COM (919) 541-5522 FTS 629-5522

8. References

deNevers, N. and Morris, J.R. "Rollback Modeling: Basic and Modified," Journal of the Air Pollution Control Association, Vol. 25, September 1975.

Wilson, J.H., Jr., "Methodologies for Projecting the Relative Air Quality Impacts of Emission Control Strategies," Presented at the 71st Annual APCA Meeting, Houston, Texas, June 25-29, 1978.

Uses, Limitations and Technical Basis of Procedures for Quantifying Relationships Between Photochemical Oxidants and Precursors, EPA-450/2-77-021a, U.S. EPA, Research Triangle Park, N.C. November 1977.

MULTIPLE POINT GAUSSIAN DISPERSION ALGORITHM WITH OPTIONAL TERRAIN ADJUSTMENT (MPTER)

1. Model Overivew: MPTER is a multiple point-source Gaussian model with optional terrain adjustments. MPTER estimates concentrations on an hour-by-hour basis for relatively inert pollutants (i.e., SO_2 and TSP). MPTER uses Pasquill-Gifford dispersion parameters and Briggs plume rise methods to calculate the spreading and the rise of plumes. The model is most applicable for source-receptor distances less than 10 kilometers and for locations with level or gently rolling terrain. Terrain adjustments are restricted to receptors whose elevation is no higher than the lowest stack top. In addition terrain adjustments options are also available for wind profile exponents, buoyancy induced dispersion, gradual plume rise, stack downwash, and plume half-life.

2. Functional Capabilities: MPTER computes hour-by-hour concentrations for relatively inert pollutants for each source-receptor pair. MPTER can handle up to 250 point sources and 180 receptors. Model users have the option of specifying the elevations and location coordinates in either metric or English units. Hourly met data can be read either off cards or off disk/tape. MPTER can calculate concentrations for averaging periods of 1, 3, 8 and 24 hours for up to a year's data. Annual concentrations can also be computed.

3. Basic Assumptions: MPTER is based upon Gaussian dispersion theory using mean meteorology conditions on an hour-by-hour basis. Dispersion coefficients used to calculate both vertical and horizontal spreading are those of Pasquill and Gifford. The rising plume is assumed to reflect completely off the top of the mixing height in neutral and unstable conditions. The plume rise is based on Briggs. MPTER can also optionally

consider stack downwash, buoyancy induced dispersion, and gradual plume rise. MPTER can either utilize constant emission rates, or hourly emission rates for each point source. The emitted pollutants should be relatively inert chemically since MPTER does not consider complex physical removal or chemical reaction processes. Users can approximate exponential decay of a pollutant by supplying a half-life. Wind speeds are extrapolated to the stack top using user supplied wind profile exponents. The optional terrain adjustment reduces the plume height relative to the ground. Additional terrain adjustment factors can be entered which control the proportion of terrain adjustment according to stability class.

4. Input and Output: Input for MPTER includes: control data, emission data, receptor information, and hourly met data. The hourly met data can be read either off cards or from a disk/tape preprocessed from surface/upper-air observations. Hourly emission data can optionally be input from disk/tape.

The variety of MPTER options allow the user to output to a printer or to write to tape information required for a multitude of applications. Tape/disk files can be written containing hourly concentrations for each receptor for each source, hourly concentrations for each receptor for all sources, concentrations for user specified averaging periods and highest five concentrations for each receptor for each averaging period. MPTER allows even more flexibility on printed output. The range of options include printouts for the highest five concentrations, for each receptor to printout for hourly contributions from each source at each receptor.

5. System Resource Requirements: MPTER is written in FORTRAN and is run on an IBM 360, CDC 6600, or Univac 1100/82. A 132 position line printer, card reader/punch, and/or tape/disk are required. A computer programming background is helpful to run the model.

6. Applications: The frequent use of MPTER is to assess air quality from multiple point sources to compare with National Ambient Air Quality Standards for SO_2 or TSP. MPTER can estimate concentrations for a single source at one or more receptors for one hour, or it can simulate concentrations on an hour-by-hour basis for as many as 250 point sources at up to 1,180 receptors for up to a year. The types of multiple applications for which MPTER is suited include stack design studies, combustion source permit applications, regulatory variances evaluation, monitoring network design, control strategy evaluation, coal conversion studies, control technology evaluation, new source review, and the prevention of significant deterioration (within 10 km).

7. Technical Contacts

D. Bruce Turner and Tom Pierce
U.S. Environmental Protection Agency
Meteorology and Assessment Division
Davis Drive
Research Triangle Park
N.C. 27711
FTS 629-4564 COM 919/541-4564

8. References

Pierce, T.E. and Turner, D.B., 1980: User's Guide for MPTER: A Multiple Point Gaussian Dispersion Algorithm with Optional Terrain Adjustment. EPA-600/8-80-016, U.S. Environmental Protection Agency, Research Triangle Park, N.C. 239 pp.

U.S. Environmental Protection Agency, 1980: MPTER tape. (Computer programs on tape containing programs, and PTPLU screening model) NTIS PB 80-168156, National Technical Information Service, Springfield, VA.

MULTI-SOURCE MODEL (CRSTER-2)

1. Model Overview: This model is basically the same as EPA's Single Source CRSTER.

2. Functional Capabilities: While essentially the same in function as CRSTER, CRSTER-2 will allow separation of multiple emission points.

3. Basic Assumptions: Same as CRSTER

4. Input and Output: Differs from CRSTER in that distinct spacial coordinates can be assigned to each point of emissions. Also, this model can handle an increased number of sources and receptors, and stack data can be input in English or metric units.

The output is basically the same as CRSTER, but stack and receptor coordinates can be output in a format for use by the CALCOMP [illegible]

5. Syst[illegible]ce Requirements: This dispersion model is written FORTRAN V. The program does not require any special software or utilities. Approximately 28K words of core memory is required to execute the model on the Univac 1110.

6. Applications: Same as CRSTER, except for added flexibility of allowing emission source separation.

7. Technical Contact

Lewis H. Nagler
Environmental Protection Agency
NOAA-Air Facilities Branch
EPA Region 4
Atlanta, GA 30365
COM 404/881-4901 FTS 257-4901

8. References

"User Information for the Modified CRSTER Program" (EPA Information Clearinghouse Files).

Environmental Protection Agency, "User's Manual for Single Source (CRSTER) Model", Publication No. EPA-450/2-77-013 (NTIS PB 271360), Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina 27711, July 1977.

NONLINEAR ROLLBACK/ROLLFORWARD MODEL

1. Model Overview: The Nonlinear Rollback/Rollforward Model considers the relationship between ozone/oxidants and single precursor hydrocarbons. It is uncoded and requires no equipment. The model can be used to provide "first cut" approximations of ambient concentrations and reductions in residual discharges in "rough" urban areas.

2. Functional Capabilities: The rollback/rollforward model considers only the relationship between ozone/oxidants and single precursor hydrocarbons. The model cannot consider combined changes in hydrocarbons and nitrogen oxides. This model can best be used to study "area wide" strategies or changes such as vehicular discharge limitations, number of automobiles, vehicle miles traveled projections. The rollback/rollforward model might be used as a "screening technique" to decide which strategies to further evaluate in a spatial and temporal photochemical model. Several variations of the model are possible: the nonlinear relationships can be developed for specific cities and specific monitoring locations within a city, a national relationship could be used, or relationships could be developed to be used for both hydrocarbons and nitrogen oxides.

3. Basic Assumptions: The Nonlinear Rollback/Rollforward Model is a stochastic model that treats ozone/oxidants as a function of hydrocarbons only. The model does not consider changing spatial and temporal patterns of residual discharges, and it assumes the same meteorological conditions as for a base case.

4. Input and Output: Input to the rollback portion of the model include ambient concentration measurements (generally hydrocarbons and oxidant/ozone) to determine nonlinear relationships. Data requirements for the rollforward portion of the model include ambient concentration measurements and projected changes in residual discharges.

Output from the model is in the form of hourly reductions in residual discharges from the rollback portion, and hourly ambient concentrations from the rollforward portion.

5. System Resource Requirements: The Nonlinear Rollback/Rollforward Model is uncoded and requires no equipment. The model user should have an understanding of the model's principles and limitations. The rollback/rollforward model itself can be developed within a few man-days from ambient monitoring data.

6. Applications: The Nonlinear Rollback/Rollforward model can be used to provide "first cut" approximations of ambient concentrations and reductions in residual discharges in "rough" ruban areas.

7. Technical Contact

Joseph Tikvart
U.S. Environmental Protection Agency
Monitoring and Data Analysis Division
Mutual Building
411 W. Chapel Hill Street
Durham, N.C. 28801
FTS 629-5561 COM 919/541-5561

8. References

Record, "Photochemical Oxidant Modeling," Vol. I, pp.32-44.

U.S. Environmental Protection Agency, Guidelines for Air Quality Maintenance, Vol. XII, pp. 21-22.

THE PLUME VISIBILITY MODEL (PLUVUE)

1. Model Overview: The design objective of the model is to calculate visual range reduction and atmospheric discoloration caused by the plumes consisting of primary particulates, nitrogen oxides, and sulfur oxides emitted by a single emissions source. The model is designed to predict the impacts of a single emissions source on visibility in Federal Class I areas. The model is a refinement of the plume model developed in the 1978 publications EPA450/378 110a, b, and c (available from NTIS) and PB 293118 set. PLUVUE predicts the transport, atmospheric diffusion, chemical conversion, optical effects, and surface deposition of point source emissions. The model uses the Gaussian formulation for transport and dispersion. The spectral radiance (intensity of light) at 39 visible wavelengths is calculated for views with and without the plume. The changes in the spectrum are used to calculate various parameters that predict the perceptibility of the plume and contrast reduction caused by the plume. PLUVUE performs plume optics calculations in a plume-based mode and an observer-based mode.

2. Functional Capabilities: The model calculates four perception parameters useful for predicting visual impact: reduction in visual range, contrast of the plume against a viewing background at the 0.55 micrometer wavelength, the blue-red ratio (color shift) of the plume, and the color change perception parameter triangle E (L*a*b*). Visibility impairment is caused by changes in light intensity as a result of light scattering and absorption in the atmosphere. Impairment can be qualified once the spectral light intensities or radiance has been calculated for the specific lines of sight of an observer at a given location in an atmosphere with known aerosol and pollutant concentrations. PLUVUE is a near-source plume visibility model, e.g., within 200 km of the source.

3. Basic Assumptions: PLUVUE is based on Gaussian atmospheric dispersion assumptions, contains Briggs' plume rise equations, allows for surface deposition during the day and contains atmospheric chemistry modules that allow for conversion of nitric oxide to nitrogen dioxide and sulfur dioxide to sulfate aerosol. Scattering and absorption properties are calculated for particles and gases. For nitrogen dioxide, the absorption at a particular wavelength is a tabulated function multiplied by the concentration. The effect of particle size on the wavelength dependence of the scattering coefficient and the phase function is calculated and the Mie equations are also solved. Calculation of light intensity follows from the radiative transfer equation.

4. Input and Output: The input data required for PLUVUE include: wind speed aloft, stability category, lapse rate mixing depth, relative humidity, sulfur dioxide, nitrous oxides and particulate emission rates, stack gas parameters, stack gas oxygen content, ambient temperature, ambient nitrous oxides, nitrogen dioxide, ozone and sulfur dioxide concentrations, properties of background and emitted aerosols in two size modes, background visual range, deposition velocities for sulfur dioxide, nitrous oxides, coarse mode and accumulation mode aerosol, UTM coordinates and elevation of the source, and UTM coordinates and elevation of the observer location.

The principal PLUVUE run output is the print file written on logical unit six. All runs have the data tables for the emissions source, meteorological and ambient air quality, and background radiative transfer. Plot files can also be written by PLUVUE. If a PLUVUE run is for either observer-based or plume-based calculations, either an observer-based or a plume-based plot file will be centered. These files are written on disk storage units.

5. System Resource Requirements: PLUVUE is written in FORTRAN. It is run on an Univac 1110 mainframe. It requires 25K bytes of core storage for execution. The model uses a printer system line printer for output. It also requires a card reader. An engineer with programming background is helpful.

6. Applications: PLUVUE has been used by EPA primarily in a research mode and to provide estimates for hypothetical scenarios such as power plant siting impact.

7. Technical Contact

James Dicke
U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Research Triangle Park
North Carolina 27711
COM 919/541-5681 FTS 629-5681

8. References

EPA, User's Manual for the Plume Visibility Model (PLUVUE), November 1980, EPA-450/4-80-032.

Latimer, D.A., et. al., The Development of Mathematical Models for the Prediction of Anthropogenic Visibility Impairment. 1978, EPA 450/3-78-110a, b, c.

Latimer, D.A., Power Plant Impacts on Visibility in the West: Siting and Emissions Control Implications. JAPCA, Vol. 30, pp. 142-146, 1980.

Bergstron, R. W., et al., "Comparison of the Observed and Predicted Visual Effects Caused by Power Plant Plumes Symposium on Plumes and Visibility," November 10-14, 1980, to be published in Atmospheric Environment, 1981.

POINT, AREA, LINE SOURCE ALGORITHM (PAL)

1. Model Overview. The Point, Area, Line Source Algorithm is a short-term Gaussian steady state algorithm that estimates concentrations of stable pollutants from point, area, and line sources. Computations from area sources include effects of the edge of the source. Line source computations can include effects from a variable emission rate along the source. The algorithm is not intended for application to entire urban areas, but for smaller scale analysis of such sources as shopping centers, airports, and single plants. Hourly concentrations are estimated and average concentrations for 1 hour to 24 hours can be obtained.

2. Functional Capabilities. Concentration estimates are given for up to 99 receptor locations, and there are concentration estimates for 6 different source types, as many as 99 sources of each type. The model provides concentration averages for 1 to 24 hours for each source type.

3. Basic Assumptions:

A. Source-Receptor Relationship. Arbitary locations are given for each point, area, and line source. Area source sizes are specified by an X and Y dimension. A horizontal finite line or curved path is utilized, as is a slant finite line. Receptor location is arbitrary. Release heights for point, area, and line sources are arbitary, as are receptor heights. A flat terrain is assumed, and the model provides a unique separation for each source-receptor pair.

B. Emission Rate. Point sources use a single rate for each source. Area sources also use a single rate for each source. Area integrations are done by numerical intergration in the up-wind direction of the concentration from an infinite crosswind line source corrected for finite length. Horizontal finite line and curved path sources assume a constant uniform emission rate for each line. Slant line and special path sources assume a variable emission rate along line or path.

C. Chemical Composition. The model does not treat this.

D. Plume Behavior. The model uses Briggs (1969, 1971, 1972) neutral/unstable formulas. If stack height plus plume rise is greater than the mixing height, ground level concentrations are assumed to be equal to zero. No plume rise calculation is performed for area or line sources, and the model does not treat fumigation or downwash.

E. Horizontal Wind Field. Arbitary wind speed and direction is user-specified. Variation of wind speed with height is optional, and a constant, uniform (steady-state) wind is assumed.

F. Vertical Wind Speed. This is assumed to be equal to zero.

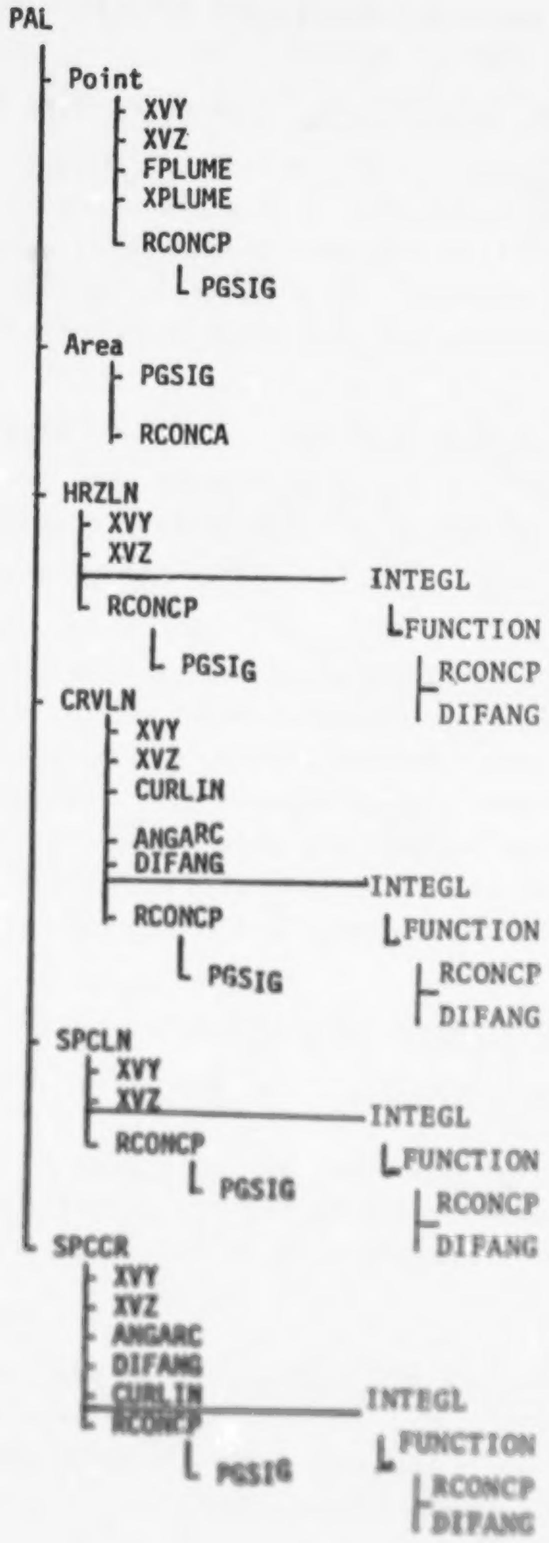
G. Horizontal Dispersion. This model uses a semi-empirical/Gaussian plume. The user specifies which of the six stability classes are to be used: Turner (1964). Dispersion coefficients are from Turner (1969). For distances less than 100m, dispersion coefficients for line sources are from Zimmerman and Thompson (1975). The initial value of the dispersion coefficient is specified by the user, and no further adjustments to the dispersion coefficients are made.

H. Chemistry/Reaction Mechanism. This is not treated.

I. Physical Removal. The model does not treat this.

4. Input and Output: The user must specify the source types and provide meteorological data. Output from the model includes hourly and average (up to 24 hour) concentrations at each receptor.

5. System Resource Requirements. This dispersion model is written in FORTRAN V. The program does not require any special software or utilities. Approximately 51K words of core are required to execute on the Univac 1110.


PAL
Point
XVY
XVZ
FPLUME
XPLUME
RCONCP
PGSIG
Area
PGSIG
RCONCA
HRZLN
XVY
XVZ
INTEGL
RCONCP
FUNCTION
PGSIG
RCONCP
CRVLN
DIFANG
XVY
XVZ
CURLIN
ANGARC
DIFANG
INTEGL
RCONCP
FUNCTION
PGSIG
RCONCP
DIFANG
SPCLN
XVY
XVZ
INTEGL
RCONCP
FUNCTION
PGSIG
RCONCP
SPCCR
DIFANG
XVY
XVZ
ANGARC
DIFANG
CURLIN
INTEGL
RCONCP
FUNCTION
PGSIG
RCONCP
DIFANG

FLOWCHART FOR PAL

6. Applications. The source program for this dispersion model is available as part of UNAMAP (Version 3), PB 277 193 for $420 from Computer Products, NTIS, Springfield, VA 22161.

7. Technical Contact

D. Bruce Turner
U.S. Environmental Protection Agency
Environmental Applications Branch
Mail Drop 80
Research Triangle Park
N.C. 27711
FTS 629-4564 COM 919/541-4564

8. References

Petersen, W.B., User's Guide for PAL, A Gaussian Plume Algorithm for Point, Area, and Line Sources, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, Environmental Monitoring Series, EPA-600/4-78-013, 1975.

Turner, D.B., and Petersen, W.B., A Gaussian Plume Algorithm for Point, Area, and Line Sources, NATO/CCMS Sixth International Technical Meeting on Air Pollution Modeling and Its Application, V 42: 185-228, 1975.

POINT SOURCE GAUSSIAN PLUME MODEL (PTPLU)

1. Model Overview: PTPLU is a point source dispersion Gaussian screening model for estimating maximum surface concentrations for 1-hour concentrations. PTPLU is based upon Briggs plume rise methods and Pasquill-Gifford dispersion coefficients as outlined in the Workbook of Atmospheric Dispersion Estimates. PTPLU is an adaptation and improvement of PTMAX which allows for wind profile exponents and other optional calculations such as bouyancy induced dispersion, stack downwash, and gradual plume rise.

PTPLU produces an analysis of concentration as a function of wind speed and stability class for both wind speeds constant with height and wind speeds increasing with height. Use of the extrapolated wind speeds and the options allows the model user a more accurate selection of distances to maximum concentration.

2. Functional Capabilities: PTPLU estimates the maximum ground-level concentration and the distance to the maximum for both wind speeds constant with height and wind speeds increasing with height for each stability class. The user has the option of selecting anemometer height, receptor height, wind profile exponents, stack downwash, buoyancy inducted dispersion, gradual plume rise, and mixing height. Output consists of 2 two-dimensional tables listing maximum concentrations, the distance to maximum concentrations, and the effective plume heights for a range of surface wind speeds and extrapolated wind speeds in each stability class.

3. Basic Assumptions: PTPLU calculates the source-receptor distance to the point of maximum concentration for each wind speed and stability class. Relatively inert pollutants are modeled and emissions are assumed to be constant. The plume is spread horizontally and vertically using P-G dispersion

coefficients. Briggs plume rise computations are employed with options available for buoyancy induced dispersion, stack downwash, and gradual plume rise. PTPLU does not allow for any depletion of the plume by physical removal or chemical reactions. Eddy reflection with the ground is assumed. If the effective plume height is calculated to be below the mixing height in neutral and unstable conditions, then multiple reflections of the plume between the ground and the mixing height are computed. But if the effective plume height is above the mixing height in neutral and unstable conditions then no calculations are made for ground-level concentrations. Also, ground-level concentrations are not calculated if the distance to maximum concentration extends beyond 100 kilometers from the source. Cautionary messages are printed for plume heights greater than 200 meters and plume resident times greater than that expected under normal atmospheric conditions.

4. Input and Output: PTPLU is extremely convenient since only nominal effort is needed to supply the necessary input. Four data cards are needed for a single run, however, additional separate point soures can be analyzed by input of two data cards for every source. Information required to run PTPLU includes selection of options, anemometer height, wind profile exponents, stack parameters (emission rate, stack height, exit velocity, stack gas temperature, and stack diameter), receptor height, and mixing height.

PTPLU is a screening model and its output results can be helpful in more detailed modeling. In particular, the tables of concentration and distance to maximum concentration can be examined for selection of receptor distances for use in detailed models.

5. System Resource Requirements: PTPLU is written in FORTRAN and can be run on IBM 360, CDC 6600, or Univac 1100/82. Approximately 12K bytes of core memory are needed for execution on the Univac 1100/82. A 132 position line printer is required. Manpower needs include an operator with knowledge of computer programming.

6. Applications: PTPLU is being used to screen maximum hourly concentrations of various meteorological conditions.

7. Technical Contact

Tom Pierce
U.S. Environmental Protection Agency
Environmental Operations Branch
Mail Drop 80
Research Triangle Park
N.C. 27711
COM (919) 541-4564 FTS 629-4564

8. References

The PTPLU source program is presently available on the MPTER tape from COMPUTER PRODUCTS, NTIS, Springfield, VA. 22161. Ask for PB80-168156; the price is $420. The PTPLU program is also available on UNAMAP (version 4).

Preparation of a user's guide is underway, and the user's guide should be available by October 1981.

POINT SOURCE MODELS (PTMAX, PTDIS, & PTMTP)

1. Model Overview: These point source models use Briggs plume rise methods and Pasquill-Gifford dispersion methods as given in EPA's AP-26, "Workbook of Atmospheric Dispersion Estimates," to estimate hourly concentrations for stable pollutants.

PTMAX is an interactive program that performs an analysis of the maximum short-term concentrations from a single point source as a function of stability and wind speed. The final plume height is used for each computation.

PTDIS is an interactive program that estimates short-term concentrations directly downwind of a point source at distances specified by the user. The effect of limiting vertical dispersion by a mixing height can be included and gradual plume rise to the point of final rise is also considered. An option allows the calculation of isopleth half-widths for specific concentrations at each downwind distance.

PTMTP is an interactive program that estimates for a number of arbitrarily located receptor points at or above ground-level, the concentration from a number of point sources. Plume rise is determined for each source. Downwind and crosswind distances are determined for each source-receptor pair. Concentrations at a receptor from various sources are assumed additive. Hourly meteorological data are used; both hourly concentrations and averages over any averaging time from one to 24 hours can be obtained.

2. Functional Capabilities: PTMAX estimates maximum ground-level concentration and distance to maximum for combinations of stability class and wind sped (internal to program).

Output from the model is a two-dimensional table giving maximum concentration, distance to maximum, and height of final rise for each stability-wind speed combination.

PTDIS estimates the ground-level concentrations directly downwind of source for each downwind distance specified (maximum number of distances is equal to 50) for one set of specified meteorological conditions. A table is produced with distance, height of plume, and ground-level concentration given for each distance. The program may reiterate for additional meteorological conditions in the same run, or for additional source and meteorology in the same run.

PTMTP estimates concentrations at arbitrary heights above ground for multiple sources at multiple receptors for multiple hourly time periods. Input data is repeated in tabular form. Total concentrations at each receptor and concentration contribution from each source may be tabulated hourly. Average concentrations (maximum 24 hours) are given for each receptor. The concentration contribution from each source for averaging time is optional.

3. Basic Assumptions:

A. Source-Receptor Relationship. For PTMAX all receptor locations are determined internally for a point of maximum. For PTDIS all receptors are considered directly downwind of the plume. For PTMTP each source and receptor is arbitrarily located by coordinates in a kilometer grid scheme.

B. Emission Rate. A single constant emission rate for each source is assumed.

C. Chemical Composition. The models treat chemical composition as a single inert pollutant.

D. Plume Behavior. Gaussian spreading is both horizontal and vertical. Briggs (1969, 1971, 1972) plume rise formulas are used. Eddy reflection from the ground in all three models is assumed, and multiple eddy reflections from the ground and mixing height are used in PTDIS and PTMTP. If the plume height exceeds the mixing height, the ground-level concentration is assumed to be zero.

E. Horizontal Wind Field. The wind speed is internal in PTMAX, and it is user-specified in PTDIS. The wind speed and direction are user-specified in PTMTP.

F. Vertical Wind Speed. This is assumed to be equal to zero.

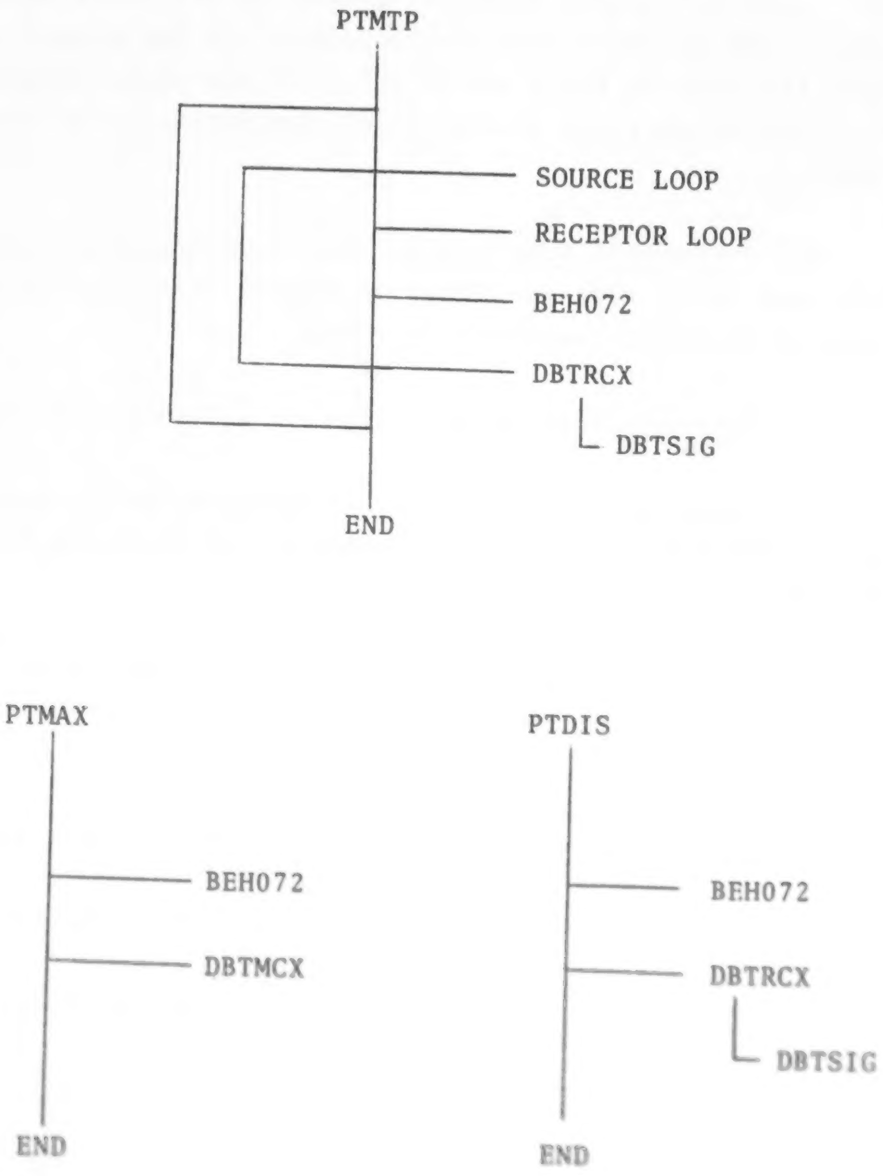
G. Horizontal Dispersion. A Gaussian horizontal plume shape is assumed. Dispersion parameters of Pasquill-Gifford are dependent upon stability class.

H. Vertical Dispersion. A Gaussian plume shape is assumed. Dispersion parameters of Pasquill-Gifford are dependent upon stability class.

I. Chemistry/Reaction Mechanism. This is not treated.

J. Physical Removal. This is not treated by the models.

K. Background. This is not treated by the models.


PTMTP
SOURCE LOOP
RECEPTOR LOOP
BEH072
DBTRCX
DBTSIG
END
PTMAX
BEH072
DBTMCX
END
PTDIS
BEH072
DBTRCX
DBTSIG
END

SIMPLIFIED FLOWCHARTS FOR PTMAX, PTDIS, AND PTMTP

4. Input and Output: PTMAX has the ability to run additional sources in the same run. PTDIS can run additional meteorological or additional sources and meteorology or other distances, additional sources and meteorology in the same run. PTMTP has optional output for hourly periods and for concentration contribution from each source for averaging time. It can run for additional meteorology or additional receptors, and meteorology in the same run. This model, which gives estimates for a single point, would not normally be calibrated or verified in actual application, but rather would be used for planning or design purposes to find a "worst case" impact.

5. System Resource Requirements: This dispersion model is written in FORTRAN V. The program does not require any special software or utilities. Approximately 12K words of core memory are required to execute on the Univac 1110.

6. Applications: The source program for this dispersion model is available as part of UNAMAP (Version 3), PB 277 193, for $420 from Computer Products, NTIS, Springfield, VA 22161.

7. Technical Contact

D. Bruce Turner
U.S. Environmental Protection Agency
Mail Drop 80
Environmental Appplications Branch
Research Triangle Park, NC 27711
FTS 629-4564 COM 919/541-4564

8. Reference

Turner, D.B., and Busse, A.D., Users' Guides to the Interactive Versions of Three Point Source Dispersion Programs: PTMAX, PTDIS, and PTMTP, Preliminary Draft, Meteorology Laboratory, U.S. Environmental Protection Agency. Research Triangle Park, NC 27711, 1973.

REACTIVE PLUME MODEL (RPM-II)

1. Model Overview: The Reactive Plume Model (RPM-II) is an air quality simulation model that provides a time history of pollutant concentrations within a chemically reactive point source plume. Its purpose is to estimate the concentration levels these species will attain within the plume downwind of the source by simulating in the model the physical and chemical processes responsible for the plume's evolution. These include the emissions of primary pollutants from the source, their transport and dispersion downwind, their chemical transformation into secondary products, and the entrainment of background ambient air into the plume. Simulated species of particular interest would include NO, NO_2, and O_3. RPM-II was developed and tested by Systems Applicators, Inc. (SAI) of San Rafael, California, for the Environmental Protection Agency.

2. Functional Capabilities: RPM-II simulates the reactive system of NO_x-HC-O_3 species with the Carbon Bond-II generalized kinetic mechanism. This includes a set of 68 chemical reactions with 35 separate species, including NO, NO_2, O_3, six classes of organics, PAN, CO, and other intermediate products. The model is constructed within a Lagrangian framework. The plume parcel is followed downwind from the source as it is advected by the wind. The frame of reference moves with the parcel. The plume model is composed of a fixed number of cross-wind cells, typically from 2 to 10, that can expand as they move downwind. The rate of horizontal dispersion is determined by Fickian diffusion considerations. The rectangular cells comprising the plume are considered well mixed reactors. The model is applicable under limited mixing atmospheric conditions and ground level computed concentrations are relevant only after the plume touch-down point has been

reached. While RPM-II is primarily designed for use as a point source plume model, an urban area plume may also be modeled by considering the source area as a virtual upwind point source. The model simulates the evolving concentrations using time steps of less than a minute, but the model inputs and outputs are hourly averages. Concentration units are in parts per million.

The model's limitations include the requirement for valid ambient concentration estimates of reactants along the plume trajectory, and the specification of valid wind speeds and dispersion rates, especially in complex terrain applications.

3. Basic Assumptions: The plume is assumed to advect downwind of the source according to the specified hour averaged wind speed and direction. Fickian dispersion is assumed to govern the diffusion between adjacent cells in the model and all cells are assumed to be well mixed. The numerical solution of the set of chemical reactions is by a modified version of the GEAR routine, a predictor - corrector method for stiff systems of differential equations. It is implicitly assumed that the Carbon Bond-II mechanism is an accurate description of the chemical transformations of NO_x-HC-O_3 in the real atmosphere.

4. Input and Output: Inputs to the model include: wind speed and dispersion rates as a function of time and downwind distance respectively; average initial concentrations for all species and the time varying ambient concentrations (an option); hourly source emission rates; and the time varying photolysis rates for the photolysis chemical reactions. The reactions comprising the chemical kinetic mechanism are also a set of inputs.

Outputs from RPM-II include: A printout of all input data; a printout of the program control variables; a printout of plume concentrations, plume widths, plume depths, wind speed, and photolysis factors at various downwind distances; and printer plots of average plume and ambient concentrations versus time. Average concentrations are printed for each species within each plume cell as well as average concentrations for the entire plume.

5. System Resource Requirements: RPM-II is coded in FORTRAN. It can be run on an Univac 1110 mainframe or an equivalent computer. It requires about 260K bytes (65,000 words) of core for execution. The model uses any regular printer for output. Skills in programming, environmental engineering and meteorology (with a background in atmospheric chemistry) are useful.

6. Applications: This model aids in the analysis of reactive plumes from point sources. A limited data base from such sources was collected as part of the Midwest Interstate Sulfur Transport and Transformation (MISTT) project in and around St. Louis in 1976. SAI analyzed this data base for use with the RPM-II and applied the model to 10 test cases for the EPA. Despite problems with the ambient HC measurements in the data base, model results are encouraging.

7. Technial Contact

Kenneth L. Schere
U. S. Environmental Protection Agency
Environmental Sciences Research Laboratory
Mail Drop 80
Research Triangle Park
N.C. 27711
COM 919/541-3795 FTS 629-3795

8. References

Yocke, M.S., Stewart, D.A., Liu, M.K., and Burton, C. S. 1980: Evaluation of RPM-II and Simple Short-Term NO_2 Model Predictions Using MISTT Data. Proc. of Second Joint Conference on Applications of Air Pollution Meterology, New Orleans, LA, March 1980.

Liu, M., Stewart, D. A., and Roth, P.M. 1978: An Improved Version of the Reactive Plume Model (RPM-II). Paper presented at the Ninth NATO/CCMS International Technical Meeting on Air Pollution Modeling, Toronto, Canada, August 1978.

REGIONAL EMISSIONS PROJECTION SYSTEM (REPS)

1. Model Overview: The REPS model is a series of FORTRAN and PL/1 programs that utilize data on existing air pollution sources and projected energy use to project emissions (and proxy air quality measures) for five of the criteria pollutants (oxidants and lead are excluded) for the 243 Air Quality Control Regions (AQCR's) in the United States. The model was originally developed by the U.S. Environmental Protection Agency; the revised model is available from the Energy Information Administration of the U.S. Department of Energy.

2. Functional Capabilities: REPS permits the examination of projected emissions under changes in (1) environmental control policy, (2) projected energy use, or (3) patterns of economic growth. Ambient proxy measures of air quality are based on emission density and population exposure. Outputs can be generated in tabular form or map displays. Forecasts can be made for any year from 1980-2000.

3. Basic Assumptions: The REPS model relies on the National Emissions Data System (NEDS) for base year (1975) and estimates of future emissions from present sources. A constant annual retirement rate is applied to all AQCR's and fuel-burning source categories. Regionalization of expected growth is based on the Department of Commerce OBERS projections, the Energy Information Administration's fuel use projections, and assumptions concerning the expected patterns of fuel switching.

4. Input and Output: Major inputs are the NEDS file, OBERS projections by AQCR and fuel use projections by Federal Region. The user may also provide information on specific synthetic fuel facilities and/or information on the desired environmental control policy to develop projected regional emissions in map or tabular form.

5. System Resource Requirements: The REPS is written in FORTRAN and PL/1 and is currently operating on IBM 370 system. The programs require approximately 200K bytes and a full run can be made for less than $100. Required operator skills include programming and engineering.

6. Applications: REPS results have been used for the following:
   1) The Department of Energy report, 1985 Air Pollution Emissions, a study of the regional air emission impacts of the National Energy Plan.
   2) The environmental chapter in the Energy Information Administrator's Annual Report to Congress, 1978.
   3) Environmental analysis of elements of the proposed National Energy Supply Strategy under development by the Department of Energy.

7. Technical Contacts

William Weygandt
U.S. Department of Energy
Washington, D.C. 20461

8. References

Booz, Allen, and Hamilton. Regional Emission Projection System--System Documentation. January 1977.

Energy Information Administration. 1977 Annual Report to Congress. Volume II, April 1978.

Pechan, E.H. An Air Emissions Analysis of Energy Projections for the Annual Report to Congress, in preparation.

Pechan, E.H. 1985 Air Pollution Emissions. Department of Energy DOE/PE-0001, Government Printing Office, December 1977.

U.S. Environmental Protection Agency. AEROS Manual Series Volume I: AEROS Overview. EPA-450/2-76-001, February 1976.

U.S. Environmental Protection Agency. AEROS Manual Series Volume II: AEROS User's Manual. EPA-450/2-76-029, December 1976.

U.S. Environmental Protection Agency. AEROS Manual Series Volume V: AEROS Manual of Codes. EPA-450/2-76-005, April 1976.

U.S. Environmental Protection Agency. Compilation of Air Pollutant Emission Factors. Second Edition, AP-42, Parts A and B, February 1976.

SAI AIRSHED MODEL (SAIASP)

1. Model Overview: The SAI Airshed Model is a grid-type photochemical air quality simulation model. Its primary purpose is to estimate the evolution of concentrations of urban atmospheric smog-related pollutants, including ozone. These concentration estimates are based on simulating the physical and chemical processes occurring in the ambient atmosphere that are responsible for ozone production. These include the emissions of organics and NO_x, chemical reactions of these precursors, advection and dispersion among grid cells, and transport of ozone and its precursors into the model region from upwind areas. The precursor include NO_2, NO, and six classes of organics. Typically, a model simulation period is on the order of one day. This model is quite complex and is rather input data-intensive. Nevertheless, it is useful for providing spatial and temporal resolution of ozone concentration estimates based on a detailed consideration of the underlying physical and chemical processes.

2. Functional Capabilties: The model considers emissions, the atmospheric chemistry of ozone formation, advection, and dispersion. The chemistry embedded in the model includes 71 reactions and 35 species including NO_2, NO, six classes of organics, ozone, PAN, CO, and several intermediate products. Advection is simulated by estimating the transfer between neighboring cells, and dispersion is estimated by using horizontal and vertical diffusivity coefficients. Wind shear can also be considered. The model considers these processes in each cell of a three dimensional grid system. This grid system typically includes four to six vertical layers of between 15 x 15 and 30 x 30 cells, each cell being between two and ten

kilometers square. The model simulates the evolving concentrations using time steps of less than a minute, but the model inputs and outputs are hourly averages. The principal limitations of the model are its complexity and the substantial amount of data required.

3. Basic Assumptions: The SAI Airshed Model uses a finite difference method to calculate the progression of pollutant concentrations through a series of time steps. The model assumes flat terrain in estimating concentrations, although the influence of the terrain on the wind field can be considered if the user is able to do so. All emissions and concentrations are assumed uniformly mixed thoughout each grid cell. It is assumed that turbulent fluxes are linearly related to the gradients in the mean concentrations so that eddy diffusivities are used in the diffusion calculations.

4. Input and Output: The SAI Airshed Model requires various emissions, and meteorological and air quality data for each grid cell in the grid system. The emissions inventory must be gridded hourly, and must include NO_2, NO, and five classes of organics. The meteorological and air quality input data are interpolated from the values measured by a relatively dense monitoring network. The meteorological data include wind speed; wind direction; mixing height; atmospheric stability and photolysis rate constant; and air quality data including concentrations of NO_x, organics, and ozone at the beginning of the simulation and at the upwind boundary. If an inert pollutant is being simulated, only data for that pollutant is necessary.

The principal output of the model is a printed array of concentrations at ground-level or any level aloft throughout the grid for each hour for each major pollutant. This array of concentrations is also put into disk storage in case the user wishes to develop programs to analyze the data further. In addition, the model provides the option of estimating concentrations at specific sites by interpolating among the concentrations in the surrounding grid cells.

5. System Resource Requirements: SAIASP is coded in FORTRAN. It can be run on an Univac 1110 mainframe or an equivalent computer. The model requires about 70,000 words of core storage for execution. It uses any regular printer for output. Useful operation skills include a background in programming, engineering, and meteorology with experience in atmospheric chemistry.

6. Applications: The SAI Airshed Model has been used by EPA and some state agencies to estimate the impact of emission controls on urban ozone concentrations. The model is currently undergoing evaluation and verification as part of the EPA Regional Air Pollution Study (RAPS) model validation program. The urban area modeled in this study is St. Louis, MO.

7. Technical Contact

Kenneth L. Schere
U.S. Environmental Protection Agency
Environmental Sciences Research Laboratory
Mail Drop 80
Research Triangle Park
N.C. 27711
COM 919/541-3795 FTS 629-3795

8. References

Only draft documentation is available at this time.

SIMULATION OF HUMAN AIR POLUTION EXPOSURES (SHAPE)

1. Model Overview: The Simulation of Human Air Pollution Exposures (SHAPE) model was developed at Stanford University`s Department of Statistics in 1980-81 under an Innovative Research Program research grant (Ott, 1981). Its purpose was to provide environmental descision makers and scientists with a methodology for generating frequency distributions of human exposures to air pollution either for an urban area or for the nation as a whole. Version I of the SHAPE program, completed in May 1981, generates a frequency distribution of the population`s exposure to carbon monoxide (CO) for the U.S. population as a whole on any particular day (24-hour period) of the year that is specified by the user. It combines activity patterns of the population with statistical descriptions of pollutants concentrations in specified locations ("microenvironments") in order to calculate the diurnal pollutant exposure concentration of each person comprising the population. As each person`s diurnal exposure is computed, the program stores the maximum hourly exposure, the maximum 8-hour running average exposure, and the highest hourly blood carboxyhemoglobin (COHb) level. Then a frequency distribution is generated for each of these three variables, as well as statistical results (mean, standard deviation, minimum, maximum, etc.), and the line printer displays these results graphically. The program can be run for a variety of different assumptions about regulatory actions and changes in population activity patterns, and the impact of different control strategies or travel habits on the frequency distribution of exposures can be examined.

The program was developed as an outgrowth of earlier research that showed that fixed air monitoring stations do not accurately reflect the exposures of the population, due largely to the fact that concentrations indoors (where the public spends over 80% of its time) and in traffic (where concentrations are known to be very high) are different from those observed at fixed monitoring stations. The program will be validated with a large-scale field study using personal exposure monitors at some time in the future. At present, it provides the only means currently available for estimating the frequency distribution of thee exposures of a population, either on a national basis or an urban basis.

2. Functional Capabilities: The SHAPE program is written in FORTRAN and uses Monte Carlo simulation to calculate carbon monoxide (CO) exposures of the population. During a 24-hour period, the program assigns each person to specific "microenvironments" (for example, home, automobile, office, garage) based on probability distributions derived from activity pattern studies. The program then combines activity profiles with data on CO concentrations in specific microenvironments and urban background concentrations in order to calculate integrated exposures of a large number of persons over a 24-hour period. Instead of a Markov chain approach, both the time spent engaged in a specific activity and the transitions from one activity to another are treated as random variables that are sampled from distributions specified by the user. The time resolution of SHAPE is on a minute-by-minute basis, and activities (and concentrations) are coded into an activity vector consisting of 24 x 60 = 1440 minutes per 24-hour period. The "inverse transformation method" for generating random variables is used, so any arbitrary frequency distribution can be employed as an input to the program.

3. Basic Assumptions: The SHAPE computer program assumes that all persons are located in their homes (Microenvironment No. 1) at the first minute past midnight (12:01 a.m.), and the first time computed probabilistically is the work arrival time. Next, the home-to-work trip is computed. Both the work arrival time and the home-to-work trip time are sampled from probability distributions specified by the user. The mode by which the trip is taken (automobile, truck, bus, street car, subway, train, walk) also is determined by sampling from a probability distribution specified by the user. For all persons at work, it is assumed that lunch begins a a time that is uniformly distributed between 11:00 a.m. and 4 hours (240 minutes) after the time of arrival at work. The evening work departure time is assumed to be 9 hours (540 minutes) after the work arrival time. The person must return to home from work by the same transportation mode that they used to travel to work, and the travel time must be the same. A total of 14 microenvironments are used and the microenvironmental component of concentration is added to the background component of concentration, which comes from data from an actual air monitoring station. Within each microenvironment, pollutant concentrations are assumed to be lognormally distributed. The COHb blood levels are computed using the model of Ott and Mage (1978).

The program can be used to generate the frequency distribution of exposures of any number of persons, and many runs thus far have been for n = 400 persons. Increasing the number of persons in the computer simulation tends to increase the computing cost, so care should be exercised in determining how many people should be included in each computer simulation.

4. Input and Output: The user is required to specify the number of persons in the computer simulation and the date on which the simulation takes place. The date must correspond to one of the dates contained in the ambient CO data file provided by the user. The program contains demographic data (sex, age distributions, weight, distribution, employment categories), as well as activity pattern data (home-work travel mode probabilities, home-work trip time distribution, lunch travel mode probabilities, lunch trip time distribution, probability of parking in an indoor garage, and probabilities for shopping trips) which currently is based on U.S. Census data but which can be altered by the user. The user also must specify the geometric mean and geometric standard deviation of the lognormally distributed concentrations in each of 14 micorenvironments. The output from each run displays all the assumed parameters, and prints out the minute-by minute activity profiles and exposure profiles for the first 10 persons. Then three statistics and histograms are printed out for the highest 1-hour average CO exposure, highest 8-hour running average exposure, and highest COHb level for all people in the simulation.

5. System Resource Requirements: The SHAPE program is coded in FORTRAN and compiled on a FORTRAN IV (level G) computer. It has been run on an IBM 370 series system and requires 300K bytes of core storage, or less. About 5 man-days are required for model set-up, and calibration and verification can be done in about 2 man-days. The manpower needs include a computer programmer and an environmental engineer or statistician familiar with exposure estimation methodology, activity pattern field studies, and computer simulation. The model user must have an understanding of the sources of data for human activity pattern and time budget studies and the error present in these

studies. The user also must have an understanding of the concepts behind microenvironmental modeling of human exposure to air pollution (Duan, 1981) and the stochastic properties of pollutant concentrations in selected in microenvironments.

6. Application: SHAPE can be used for air pollution risk analysis by generating exposure frequency distributions for the population. It also can be used to compare the impact on the population of different vehicular emission control strategies. Finally, it can be used for planning personal monitoring field studies.

7. Technical Contact:

Wayne Ott
U.S. Environmental Protection Agency
Office of Research and Development
Office of Monitoring Systems and Quality Assurance
401 M Street, S.W.
Washington, D.C. 20460
COM 202/426-4153 FTS 426-4153

8. References:

Duan, Naihua "Micro-environment types: A Model for Human Exposure to Air Pollution," Department of Health and Human Services, Report No. WD-908-1-HHS, RAND, Santa Monica, CA, 1981.

Ott, Wayne "Exposure Estimates Based on Computer Generated Activity Patterns," Paper No. 81-57.6 presented at the 74th Annual Meeting of the Air Pollution Control Association, Philadelphia, PA, 1981.

Ott, Wayne and Mage, David, "Interpreting Urban Carbon Monoxide Concentrations by Means of a Computerized Blood COHb Model," Journal of the Air Pollution Control Association, Vol. 28, No. 9, pp. 911-916, 1978.

SINGLE SOURCE MODEL (CRSTER)

1. Model Overview: This algorithm estimates ground-level concentrations resulting from up to 19 colocated elevated stack emissions for an entire year and prints out the highest and second-highest 1-hour, 3-hour, and 24-hour concentrations as well as the annual mean concentrations at a set of 180 receptors (5 distances by 36 azimuth). The algorithm is based on a modified form of the steady-state Gaussian plume equation which uses empirical dispersion coefficients and includes adjustments for plume rise and limited mixing. Terrain adjustments are made as long as the surrounding terrain is physically lower than the lowest stack height input. Pollutant concentrations for each averaging time are computed for discrete, non-overlapping time periods (no running averages are computed) using measured hourly values of wind speed and direction, and estimated hourly values of atmospheric stability and mixing height.

2. Functional Capabilities: Concentrations are estimated for each hour of a one-year period of record at a 180-receptor grid laid out in polar coordinate form (36 directions by 5 distances) resulting from a single plant which may consist of from one to eighteen individual stacks. Sources are all colocated, that is, distances between sources are not considered. It is assumed that this algorithm will be applied to elevated sources and distances far enough away (near maximum concentrations) so that final plume rise is applicable and distances between sources will be unimportant. Output consists of tables giving concentration estimates for each receptor. Annual concentrations, highest and second highest 1-hour,

3-hour, and 24-hour concentrations are standard output. Calculations for highest and second highest for a selected averaging time of 2, 4, 6, 8, or 12 hours can be optionally selected.

3. Basic Assumptions:

Source Receptor Relationship. Up to 19 point sources, but no area sources can be run. All point sources are assumed to be at the same location, and a unique stack height is assumed to each source. Receptor locations are restricted to 36 azimuths (every 10 degrees) and 5 user-specified radial distances. There is a unique topographic elevation for each receptor which must be below the top of the stack.

Emission Rate. The model assumes a unique average emission rate for each source, and monthly variations in the emission rate are allowed.

Chemical Composition. This is treated as a single inert pollutant.

Plume Behavior. The model uses Briggs (8,) (9,) (10) final plume rise formulas, and does not treat fumigation or downwash. If the plume height exceeds the mixing height, concentrations further downwind are assumed to be equal to zero.

Horizontal Wind Field. The model uses user-supplied hourly wind direction (nearest 10 degrees), internally modified by the addition of a random integer value between -4 degrees and +5 degrees. Wind speeds are corrected for release height based on power law variations and exponents from DeMarrais(6). Different exponents are used for different stability classes, and the reference height is equal to 10 meters. A constant, uniform (steady-state) wind is assumed within each hour.

Vertical Wind Speed. This is assumed to be equal to zero.

Horizontal Dispersion. The model assumes a semiempirical/Gaussian plume. Seven stability classes are used: Turner Class 7 is an extremely stable, elevated plume assumed not to touch the ground. Dispersion coefficients are from Turner, and no further adjustments are made for variations in surface roughness, transport, or averaging time.

Vertical Dispersion. A semi-empirical/Gaussian plume is used, and the model utilizes seven stabiltiy classes. Dispersion coefficients are from Turner, and no further adjustments are made.

Chemistry/Reaction Mechanism. This is not treated.

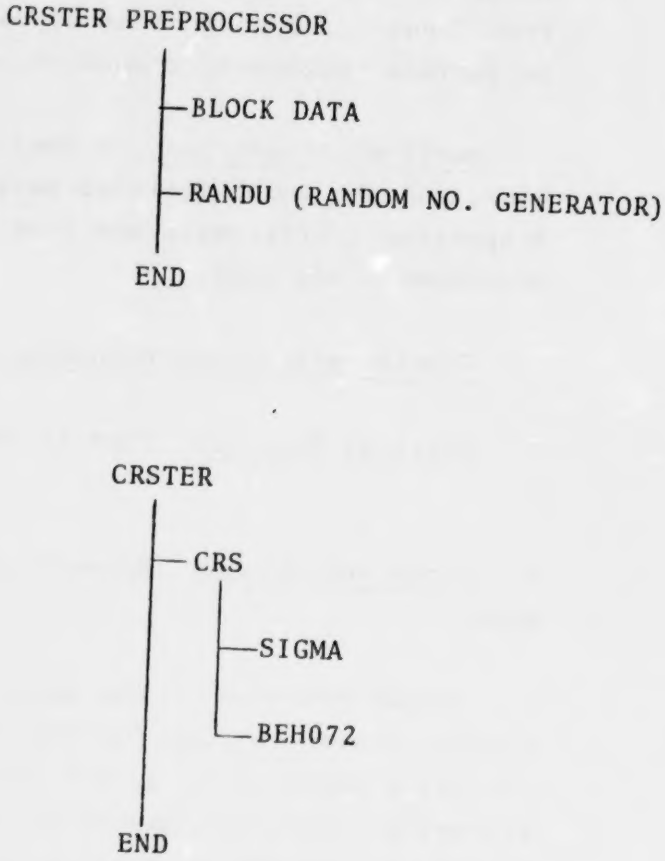
Physical Removal. This is not treated.

4. Input and Output: Meteorological data must be input to the model.

Output produced by the model includes highest and second highest concentrations for the year at each receptor for averaging times of 1, 3, and 24-hours, plus a user selected averaging time which may be 2, 4, 6, 8, or 12-hours. An annual arithmetic average at each receptor is given, and the model provides the highest 1-hour and 24-hour concentrations over the receptor field for each day, and hourly concentrations for each receptor on magnetic tape.

5. Systems Resource Requirements:

This model is coded in FORTRAN V and is run on an Univac 1110 mainframe. The model uses 28K words of core memory for execution.


CRSTER PREPROCESSOR
BLOCK DATA
RANDU (RANDOM NO. GENERATOR)
END
CRSTER
CRS
SIGMA
BEH072
END

CRSTER FLOWCHART

6. Applications: The source program for this dispersion model is available as part of UNAMAP (Version 3), PB 277 193, for $420 from Computer Products, NTIS, Springfield, Va. 22161.

7. Technical Contact

D. Bruce Turner
U.S. Environmental Protection Agency
Environmental Applications Branch
Mail Drop 80
Research Triangle Park
N.C. 27711
COM 919/541-4564 FTS 629-4564

8. References

Environmental Protection Agency, "User's Manual for Single Source (CRSTER) Model," Publication No. EPA-450/2-77-013 (NTIS PB 271360), Office of Air Quality Planning and Standards, Research Triangle Park, North Carolina 27711, July, 1977.

SYSTEMS APPLICATIONS, INC. MODEL (SAI)

1. Model Overview: The Systems Applications, Inc. (SAI) Model is a three-dimensional, dynamic air model used in the evaluation of area sources in urban areas of all terrain types. The model was designed to treat the physical processes of both transport and diffusion, and to simulate photochemical oxidation reactions. The daytime build-up of photochemical oxidants, hourly variations in ozone, and their precursors is handled by a short term application of the SAI model. The model is appropriate for examining areas ranging from very localized vicinities to whole urban areas.

2. Functional Capabilities: The model is capable of simulating photochemical oxidation reactions and the physical processes of both transport and diffusion. It incorporates user-specified multiple layer discretization and a 25 x 25 grid spacing, which is also user-specified. A fixed horizontal diffusion coefficient detracts from the actuality of the model, but the input variations in wind speed and direction add realism to the representiveness of the prototype system. The SAI model has a sensitivity to residual discharges, initial conditions, and boundary conditions, but it does provide a detailed treatment of both chemical reactions and area-wide meteorological conditions. The model is limited by its complexity, data requirements, and the modifications that are required to eliminate its "site specific" features.

3. Basic Assumptions: The SAI model is a deterministic model that is numerically integrated by the finite difference method. Constituents are assumed to be in a dynamic state.

4. Input and Output: Input for the initial set-up and calibration of the model include: activity data and residual discharge data for point and area sources; meteorological data at multiple points (wind speed, wind direction, and mixing heights); and multiple point ambient concentration data. Data requirements for verification of the model include the above meteorological data and ambient concentration data.

Output from the SAI model include ambient concentration values given at grid areas and interpolated points. The output is given in the following forms: printed hourly-averaged ground level concentration maps; printed summaries of hourly-averaged concentrations at each monitoring station; printed instantaneous ground level concentration maps; and printed summaries of instantaneous vertical concentration distributions above each monitoring station.

5. System Resource Requirements: The SAI model is coded in FORTRAN IV and run on an IBM 370/155, or equivalent. Manpower needs for the model include: a computer programmer, a research assistant, and an experienced modeler with knowledge of FORTRAN IV, the diffusion model, photochemistry, and advanced mathematical and solution techniques.

6. Applications: The SAI model can be used in the evaluation of area sources in urban areas of all terrain types.

7. Technical Contact

Joseph Tikvart
U.S. Environmental Protection Agency
Monitoring and Data Analysis Division
Mutual Building
411 W. Chapel Hill Street
Durham, N.C. 28801
FTS 629-5561 COM 919/541-5561

8. References

Record, "Photochemical Oxidant Modeling," Vol. I, pp. 92-100.

Reynolds, J.D., *et al*., "Mathematical Modeling of Photochemical Air Pollution - I, Formulation of the Model," *Atmospheric Environment*, Vol. VII (1973), pp. 1033-1061.

Reynolds, J.D., *et al*., "Mathematical Modeling of Photochemical Air Pollution - III, Evaluation of the Model," *Atmospheric Environment*, Vol. VIII (1974), pp. 563-596.

Roth, P.M., "Summary of Results of the Denver Air Quality Simulation Study: Model Evaluation and Analysis," U.S. Environmental Protection Agency, Region VIII, (February 1977).

TEXAS CLIMATOLOGICAL MODEL VERSION 2 (TCM-2)

1. Model Overview: The Texas Climatological Model Version 2 (TCM-2) uses the steady-state Gaussian plume hypothesis. It is a relatively fast FORTRAN computer program used to predict ground level, long-term concentrations of atmospheric pollutants. The Briggs plume rise, the Pasquill-Gifford-Turner dispersion equations, and sector averaging are used in this model. Contributions from area sources are determined by a modification of the method developed by Gifford-Hanna. An emissions inventory and a set of meteorological conditions are input to the model by the user. The TCM was developed by the Texas Air Control Board, Austin, Texas.

2. Functional Capabilities: Concentrations for one or two pollutants may be determined for long averaging times. Any number of area and point sources may be analyzed. Concentrations are calculated for up to 2500 locations in a user-defined rectilinear array of receptors. Up to 5 sets of meteorological conditions in the form of a meteorlogical joint frequency function and average ambient temperature may be input to the model. Important user options are exponential pollutant decay, use of only final plume rise, choice of urban or rural dispersion, and calibration with observed concentrations. A variety of other input and output options are available to enhance the utility of the model.

3. Basic Assumptions: The basic assumptions are:

   a) The Emission Rate - is constant for each set of meteorological conditions.

b) Wind Speed - The pollutants are transported downwind at an appropriate average wind speed. Wind speed is adjusted to physical stack height.

c) Wind Shear - There is no directional wind shear in the vertical.

d) Plume Behavior - The plume is infinite with no plume history. The plume is reflected at the earth's surface with no pollutant losses due to reaction or deposition at the surface.

e) Chemistry/Reaction Mechanisms - The pollutants are non-reactive gases or aerosols and remain suspended in the air following the turbulent movement of the atmosphere. There is an option to use exponential decay of pollutant concentration based upon a user input half life.

f) Horizontal and Vertical Dispersion - The concentration in the vertical direction is described by a Gaussian distribution about the plume centerline. Dispersion coefficients are from Pasquill-Gifford-Turner with no additional adjustments being made for variations in surface roughness. Horizontal dispersion is described by sector averaging instead of by a Guassian distribution. A meteorological joint frequency function is used to describe dispersion in the horizontal.

4. Input and Output:

A. Inputs to the TCM-2 are as follows:

1) Control parameters cards specify the input and output options, grid spacing, and orientation, etc.

2) Calibration factor cards

3) Meteorological joint frequency function value cards

4) Area source inventory cards

5) Point source inventory cards

6) Monitoring data cards

B. Input options

1) Point source inventory parameters may be in metric or English units.
2) Point source inventory may be read from cards or disk file.
3) Meteorological joint frequency function may be read from cards or disk file.

TCM2-s output options are:

1) A list of coordinates and concentration at each grid receptor

2) An array map of grid coordinates and concentration

3) A culpability list identifying the highest five major concentration contributors and respective contributions

4) A list of the point of maximum concentration for each scenario

5) Card punch output for input to contour plotting programs

5. System Resource Requirements: TCM-2 is coded in FORTRAN and is run on a Burroughs 6810/11 mainframe computer. It requires 17K words of core memory for execution. It uses a Burroughs B 9247-15 printer for output and a card reader/punch for input. A background in engineering, meteorology, and air pollution is useful.

6. Applications: TCM-2 is used by state air pollution control agencies, meteorological consultants, and industry for:

1) Stack parameter design studies

2) Evaluation of the impact of new sources or source modification for permit application review

3) Fuel conversion studies

4) Monitoring network design

5) Control technology evaluation

6) Control strategy evaluation for SIP

7) Prevention of significant deterioration

7. Technical Contacts

Bruce Turner
U.S. Environmental Protection Agency
Mail Drop 80
Research Triangle Park
N.C. 27711
COM 919/541-4564 FTS 629-4564

Cyril Durrenberger and James Bryant
Texas Air Control Board
Permits Section
6330 Highway 290 East
Austin, Texas 78723
COM 512/451-5711

8. References

Texas Air Control Board. "User's Guide to the Texas Climatological Model." Austin, Texas, August 1980.

TEXAS EPISODIC MODEL VERSION 8 (TEM-8)

1. Model Overview: The Texas Episodic Model Version 8 (TEM-8) uses the steady state Gaussian plume hypothesis in a FORTRAN computer program designed to predict ground level, short-term concentrations of atmospheric pollutants. The Briggs plume rise and the Pasquill-Gifford-Turner dispersion equations are used in the model. Concentrations from area sources are determined using the method developed by Gifford-Hanna. An emissions inventory and a set of meteorological conditions are input to the model by the user. The TEM was developed by the Texas Air Control Board, Austin, Texas.

2. Functional Capabilities: Concentrations for one or two pollutants may be determined for time periods from 10 minutes to 24 hours. The model, as supplied, may analyze up to 300 individual point sources and up to 50 area sources, but these size limits are easily expanded. Concentrations are calculated at up to 2500 locations in a user-defined rectilinear array of receptors. An automatic grid feature in the program may be used to define a grid that encompasses the point of maximum concentration. A variety of input and output options are available to enhance the utility of the model. Up to 24 sets of meteorological conditions may be input to the model. Exponential decay of pollutant concentration may be calculated as a user option.

3. Basic Assumptions:

   a) Emission Rate: The emission rate is constant.

   b) Wind Speed: The pollutants are transported downwind at an appropriate average wind speed. Wind speed is adjusted according to the physical stack height.

c) Wind Shear: There is no directional wind shear in the vertical.

d) Plume Behavior: The plume is infinite with no plume history. The plume is reflected at the earth's surface with no pollutant losses due to reaction or deposition at the surface.

e) Chemistry/Reaction Mechanism: The pollutants are non-reactive gases or aerosols and remain suspended in the air following the turbulent movement of the atmosphere. There is an option to use exponential decay of pollutants concentration based upon a user input half life.

f) Horizontal and Vertical Dispersion: Dispersion occurring in the downwind direction is negligible compared to advection. The concentrations in both the crosswind and the vertical directions are described by the Gaussian distribution about the plume centerline. Dispersion coefficients are from Pasquill-Gifford -Turner with no additional adjustments being made for variations in surface roughness. Horizontal coefficients (sigma-y) are assumed to represent dispersion over a 10 minute averaging period and are increased for longer averaging times to represent the greater horizontal plume meander due to fluctuations in wind direction.

4. Input and Output: Input to the TEM-8 consists of 4 types of parameter cards. Control parameter cards indicate the input and output options, the grid spacing, and orientation, etc. Scenario parameter cards indicate meterological conditions. The third and fourth cards are point and area source inventory cards. Additionally, two options are available for point source inventory cards. Parameters may be either metric or English units and they may be read from cards or disk file.

Output options include the following:

1) A list of coordinates and concentrations at each grid receptor

2) An array map of grid coordinates and concentrations

3) A culpability list identifying the five highest major concentrations contributors and their respective contributions

4) A list of the point of maximum concentrations for each scenario

5) Card punch output for input to a contour plotting program

5. System Resource Requirements:

This model is written in FORTRAN. It requires approximately 26K bytes on a Burroughs B6810/11. An engineering background with knowledge of meteorology and air pollution is helpful.

6. Applications: This model is used by state air pollution control agencies, meteorological consultants and industry for:

1) Stack parameter design studies

2) Evaluation of the impact of new source or source modifications for permit applications review

3) Fuel conversion studies

4) Monitoring network design

5. Control technology evaluation

6. Control strategy evaluation for SIP

7. Prevention of significant deterioration

7. Technical Contacts

Bruce Turner
U.S. Environmental Protection Agency
Environmental Applications Branch
Mail Drop 80
Research Triangle Park
N.C. 27711
COM 919/541-4564 FTS 629-4564

Keith Zimmerman and James Bryant
Texas Air Control Board
Permits Section
6330 Highway 290 East
Austin, Texas 78723
512/451-5711

8. References

Texas Air Control Board, "User's Guide to the Texas Episodic Model", Austin, Texas, October 1979.

Dames and Moore, "Final Report Phase I Bay Area Sulphur Oxides Study for Bay Area Air Quality Management District." October 1979.

ABATEMENT AND RESIDUAL FORECASTING MODEL (ABTRES)

1. Model Overview: The Abatement and Residual Forecasting Model (ABTRES) forecasts and reports the costs associated with pollution control systems, and the concomitant residual levels. The system is based upon "sectors"; that is, processes or technologies that have identifiable pollution control costs. These sectors are aggregated to "chapters" for reporting purposes. Chapters are industrial segments, organized in a manner determined by the analyst. This aggregation is useful since there are often several sequential operations within an industry, each with separate pollution control systems, or an industry may be defined in a general manner, to include several different end products, such as "Organic Chemicals."

2. Functional Capabilities: The ABTRES model allows the user to compute costs associated with meeting the pollution control standards in effect through internal calculations based upon certain input parameters, or the user may enter these costs exogenously. In conjunction with these cost forecasts, the model projects estimated residual levels associated with the treatment methods of each abatement technology sector. There are two standards which apply to existing industries to meet Federal guidelines for water pollution control, and these are the Best Practicable Technology (BPT) and the Best Available Technology (BAT). There are separate standards promulgated for plants established after a particular date (which varies by industry), and the set of records is referred to as New Source Performance Standards (NSPS). Sectors dealing with air pollution have a single standard to implement, which is based upon state implementation plans (SIP). There are also more stringent

regulations dealing with new plants. Types of pollution considered by the model include: particulates, sulfur oxides, nitrogen oxides, hydrocarbons, carbon monoxides, vinyl chloride, other gases and mists, biological oxygen demand, chemical oxygen demand, suspended solids, dissolved solids, acids, bases, and oils and greases.

3. Basic Assumptions: ABTRES is an accounting model that subcategorizes industries and computes costs associated with meeting the pollution control standards in effect through internal calculations based upon certain input parameters. Costs may also be entered exogenously. A straight line interpolation method is used to find the growth rates for years not specified as corresponding to these rates. Growth is held constant for the intervals between interpolation years. The conceptual growth curves are smooth; for computational purposes, the step curve is used, allocating all growth to the beginning of the fiscal year.

4. Input and Output: Input to the model is in card image form and the following types of information are included: abatement technology description, number of residuals, equipment life, interest rates, exogenous costs, loading factors, capacity utilization, number of plants, average capacity, growth percentage by interpolation year, percentage of capacity pretreating wastes prior to municipal treatment by interpolation year, residual codes for pollution types, base residual coefficients (to yield total pollutant level generated without any treatment), and fraction of waste treated.

Once forecasts of costs and residuals have been generated by the computational program of ABTRES, a report generator is implemented using the output files. The costs for several abatement technology sectors are aggregated as a "chapter level".

Different reports are issued for air and water treatment systems.

5. System Resource Requirements: Two programs must be implemented in the ABTRES system. The first is a forecasting model, and the second a report generator. The model requires 100K bytes of core storage. A knowledge of programming and an awareness of the model's theory and limitations is helpful.

6. Applications: ABTRES can be used to forecast and report the cost associated with pollution control systems and the concomitant residual levels. It has been applied to manufacturing plants and the levels of water pollution associated with these plants.

7. Technical Contact

James Titus
U.S. Environmental Protection Agency
Economic Analysis Division
PM-220
401 M Street, S.W.
Washington, D.C. 20460
COM 202/382-2774 FTS 382-2774

8. References

Wing, B.J., Abatement and Residual Forecasting Model (ABTRES), Prepared by the Professional Services Division, Control Data Corporation, Rockville, Maryland, for the Office of Planning and Evaluation, U. S. Environmental Protection Agency, Washington, D.C., April 1977.

AIR TEST MODEL (AIRTEST)

1. Model Overview: The Air Test Model is a preprocessor to the Utility Simulation Model, which can also be used as a stand alone model. Using actual fuel and specified generation for each power plant or generating unit, it calculates the controlled and uncontrolled emission of SO_2, NO_x, and particulates for one year. In addition, the model selects the least levelized cost fuel and pollution control option to meet unit specific emissions standards.

2. Functional Capabilities: The options to meet the applicable SO_2, NO_x, and particulate standards currently include: Actual 1979 data for fuels burned in the generating unit, coal washing on a coal specific basis, low sulfur coal options for each unit, coal-blending to meet unit specific standards, wet and dry F.D.G., E.S.P.'s fabric filters, low excess air, staged combustion, fuel gas recirculation, limestone injection burners, and oil hydrodesulfurization. The Air Test Model passes each unit's low cost and fuel characteristics on to the Utility Simulation Model.

3. Basic Assumptions: AIRTEST assumes minimization of levelized cost of fuel and pollution control vs. the decision factor in selection of fuel and technology.

4. Input and Output: Input is the actual fuel and specified generation for each power plant or generating unit to be considered.

The output is the controlled and uncontrolled emissions of SO_2, NO_x and particulates; pollution control option; cost and fuel type; and cost for each unit.

5. System Resource Requirements: AIRTEST is written in FORTRAN and can be run on either a CDC 7600 or IBM mainframe. Any model line printer can be used. The operator's background should include programming and engineering.

6. Application: AIRTEST is currently being used in the Acid Rain Mitigation Strategies research program.

7. Technical Contacts

Dr. Andrew Van Horn
Teknekron Research, Inc.
2118 Milvia Street
Berkeley, California 94704
415/548-4100

Paul Schwengels
U.S. Environmental Protection Agency
Office of Research and Development
401 M Street, S.W.
Washington, D.C. 20460
COM 202/382-2577 FTS 382-2577

8. References

Bowan, Carol, Clements, Don, Moffet, Michale, and Van Horn, Andy. AIRTEST USER'S GUIDE, Nov. 1980. Teknekron Report No. (RM-60-DOE80).

AUTOMOBILE DEMAND MODEL (CARMOD)

1. Model Overview: CARMOD is a 400 equation simultaneous econometric model. The model is concerned primarily with estimating long-run levels of automobile demand. CARMOD was developed by Wharton Econometric Forecasting Associates (WEFA). The model is long-run and movements toward equilibrium are governed by a stock adjustment mechanism. CARMOD resides on the IPS/TROLL system at the Massachusetts Institute of Technology.

2. Functional Capabilities: The TROLL system allows for direct user interaction with Carmod. Simulation of any equation or the production of graphs is accomplished through simple conversation with TROLL. This system also provides for a variety of output options in addition to the printing of standard regression statistics. Econometric techniques ranging from OLS to 2SLS with autocorrelation correction procedures are readily available. CARMOD's equations were estimated using ordinary least squares.

TROLL's unique file system allows all relevant files associated with a given model to be accessed automatically by referencing the model itself. The user doesn't need to be concerned with loading data or parameters. TROLL also contains a file editor and provides for off line printing.

3. Basic Assumptions: The assumptions concerning model forecasts (baseline projection) fall into three categories; demographic trends, the economic environment, and automobile characteristics.

1. The major demographic assumptions are:

   Slow population growth: the growth-rate changes from 0.17% per annum for 1976-1985 to just over 0.3% for 1995-2000.

   Family formation outspaces population: the number of family units rises from 75.3 million in 1975 to 87.4 million in 1985 (a 1.5% per annum rate) to 100.7 million by 2000 (a 0.9% per annum rate).

Families become smaller: the proportion with five or more members falls sharply, while that for three or four remains constant.

An aging population: the percentage between 20 and 29 years of age falls, especially after 1980.

2. The key economic assumptions are:

Strong real income growth: real GNP growth in excess of 5% per annum through 1978, slowing to 2% for 1979-1980, stabilizing at around 3% per annum thereafter.

Slowing inflation: the overall GNP deflator rises at around 5.5% per annum through 1980, slowing towards 4% by 1985, and reaching 3% per annum by 2000.

Declining unemployment-rate: unemployment falls towards a 5% rate by the mid-1980's, then slowly trends towards 3% by 2000.

Slowly increasing 'real' automobile costs: operating costs are expected to outpace the overall consumer price index, especially the price of gasoline - projected to increase over 20% in 1972 prices by 1985; however, 'real' purchase prices are expected to be quite stable.

3. The auto characteristics assumptions are:

Sharply reduced weights and displacements: a major domestic downsizing program, applied to each size-class in succession, reducing curb-weights about 30%, and engine displacements about 40%, by 1990.

Efficiency improvements: technological developments are projected to yield increases in fuel efficiency totalling 11% for 1976-80; thereafter these gains are held to 1% per annum on the assumption of more stringent pollution standards.

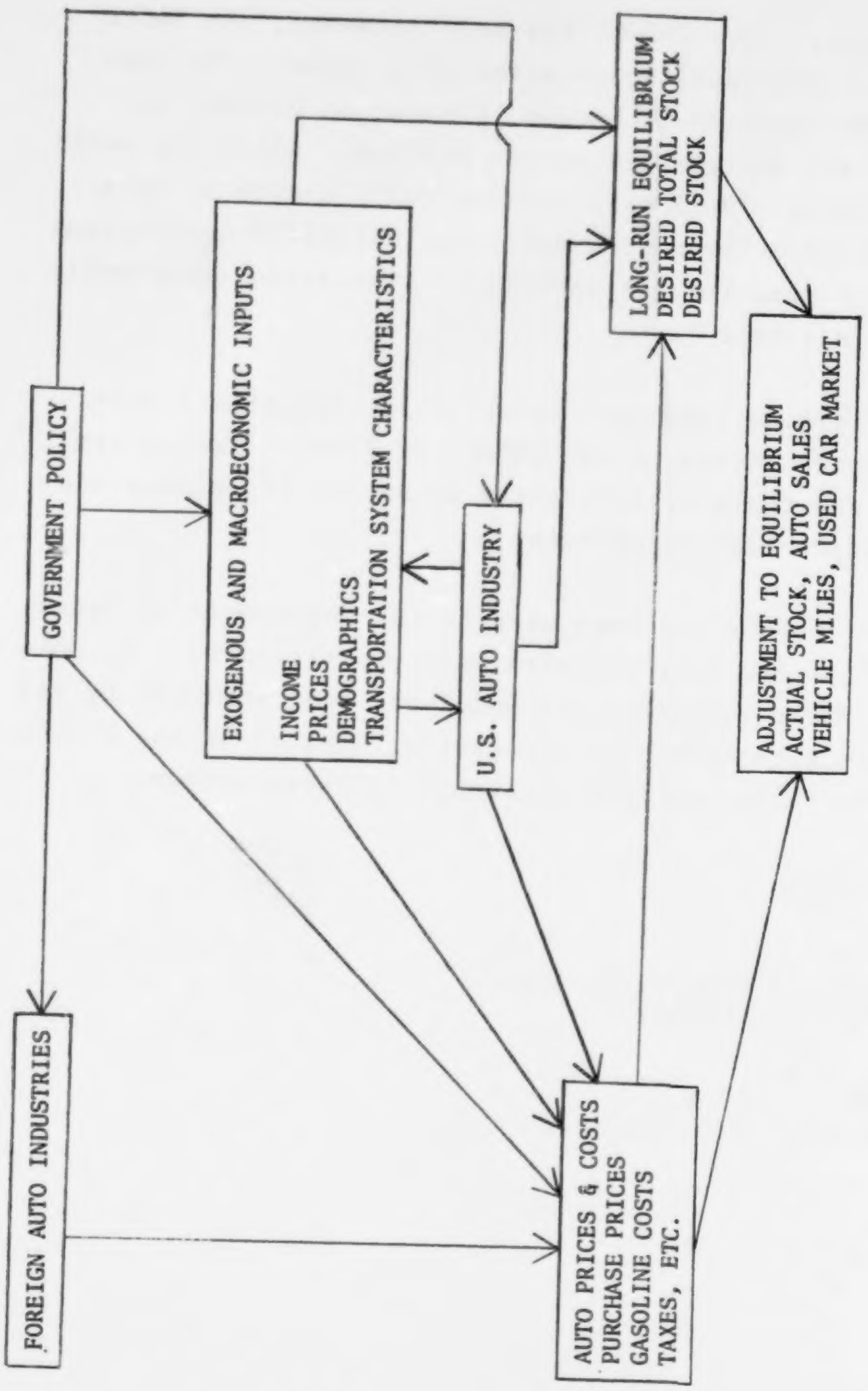
4. Input and Output: Once CARMOD has been accessed, the TROLL system automatically provides the required data input. The user can then specify the equation technique, simulation period, required statistics, and any graphic output desired. After the model has been simulated once, TROLL will automatically create a 'data set' file which includes the model, data, and estimated coefficient values. In this way performing a variety of simulation experiments at a later time is a simple task.

5. System Resource Requirements: There are no specific system resources requirements needed to run CARMOD on TROLL. The system is conversational and costs approximately $9.00 per CPU minute and $2.00 per hour connect time to operate.

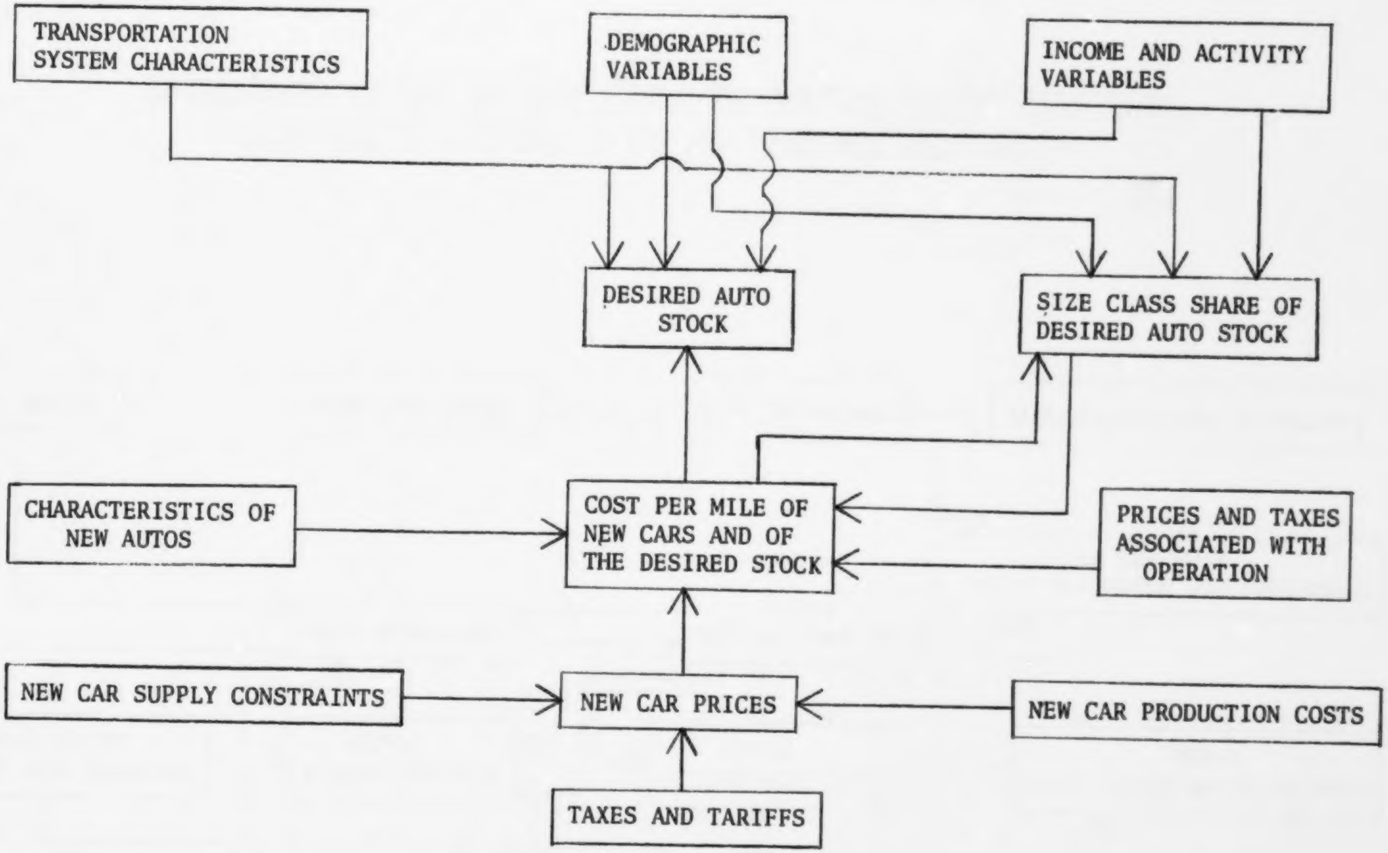
6. Applications: CARMOD has been used by the Department of Transportation to forecast the long run size and composition of U.S. auto demand and stock. More recently, the model has been employed by the Environmental Protection Agency in forecasting impacts on the U.S. automobile industry resulting from environmental regulations.

7. Technical Contacts

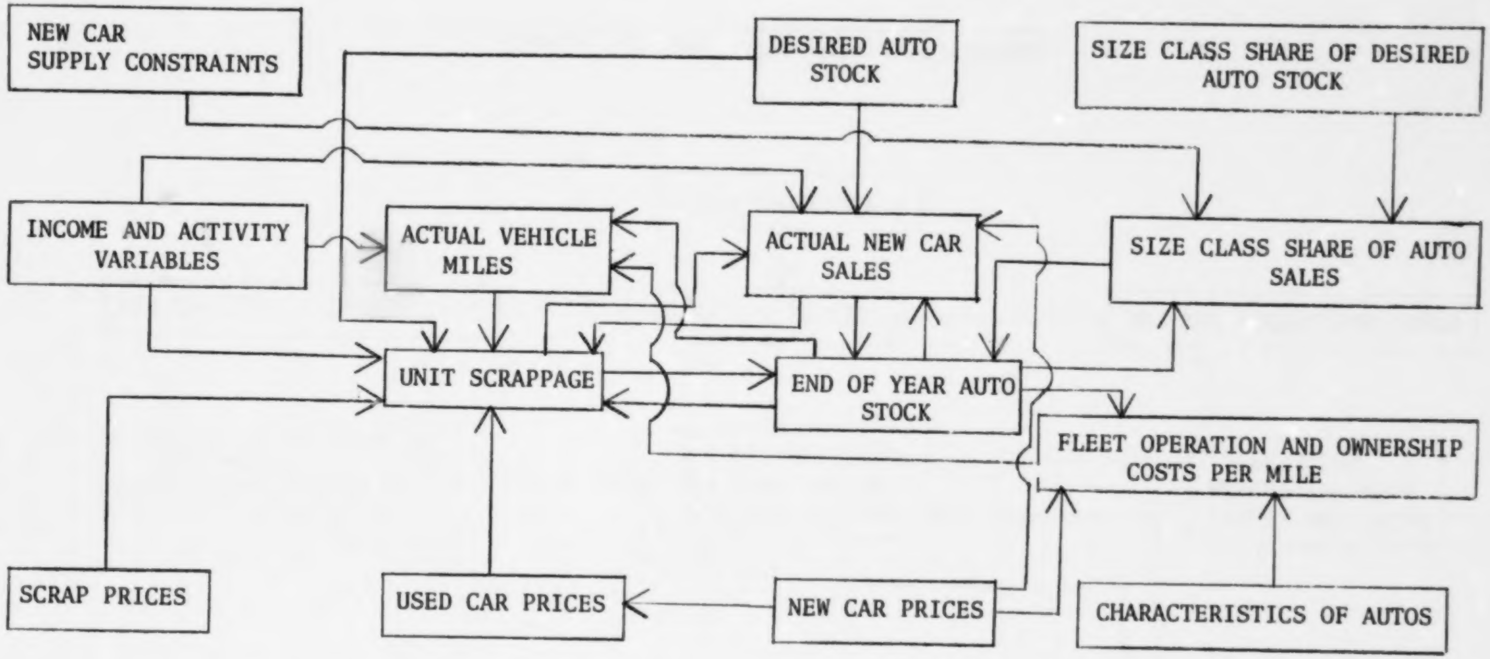
Mahesh Podar
U.S. Environmental Protection Agency
Economic Analysis Division
PM-220
401 M Street, S.W.
Washington, D.C. 20460
COM . 202/ 382-2770 FTS 382-2770


GOVERNMENT POLICY
EXOGENOUS AND MACROECONOMIC INPUTS
INCOME
PRICES
DEMOGRAPHICS
TRANSPORTATION SYSTEM CHARACTERISTICS
U.S. AUTO INDUSTRY
LONG-RUN EQUILIBRIUM
DESIRED TOTAL STOCK
DESIRED STOCK
ADJUSTMENT TO EQUILIBRIUM
ACTUAL STOCK, AUTO SALES
VEHICLE MILES, USED CAR MARKET
FOREIGN AUTO INDUSTRIES
AUTO PRICES & COSTS
PURCHASE PRICES
GASOLINE COSTS
TAXES, ETC.

SIMPLIFIED SCHEMATIC OF THE WEFA AUTO MODEL


TRANSPORTATION SYSTEM CHARACTERISTICS
DEMOGRAPHIC VARIABLES
INCOME AND ACTIVITY VARIABLES
DESIRED AUTO STOCK
SIZE CLASS SHARE OF DESIRED AUTO STOCK
CHARACTERISTICS OF NEW AUTOS
COST PER MILE OF NEW CARS AND OF THE DESIRED STOCK
PRICES AND TAXES ASSOCIATED WITH OPERATION
NEW CAR SUPPLY CONSTRAINTS
NEW CAR PRICES
NEW CAR PRODUCTION COSTS
TAXES AND TARIFFS

DETAIL OF THE LONG RUN AUTO MODEL


NEW CAR SUPPLY CONSTRAINTS
DESIRED AUTO STOCK
SIZE CLASS SHARE OF DESIRED AUTO STOCK
INCOME AND ACTIVITY VARIABLES
ACTUAL VEHICLE MILES
ACTUAL NEW CAR SALES
SIZE CLASS SHARE OF AUTO SALES
UNIT SCRAPPAGE
END OF YEAR AUTO STOCK
FLEET OPERATION AND OWNERSHIP COSTS PER MILE
SCRAP PRICES
USED CAR PRICES
NEW CAR PRICES
CHARACTERISTICS OF AUTOS

INPUT AND OUTPUT DETAIL OF THE LONG RUN AUTO MODEL:
ADJUSTMENTS TO THE DESIRED VALUES OF THE ACTIVITIES OVER TIME

8. References

Wharton Econometric Forecasting Associations, "An Analysis of the Automobile Market: Modeling the Long Run Determinants of the Demand for Automobiles" Philadelphia, PA, February 1977.

National Bureau of Economic Research, "TROLL/1 User's Guide" Cambridge, Massachusetts, June 1972.

CONSTRUCTION MODEL (CONMOD)

1. Model Overview: The construction model is an econometric model designed for the evaluation of sewer line and treatment plant expenditures by the Environmental Protection Agency. The model estimates impacts on labor supply, investment, and prices from EPA sewer-related expenditures. CONMOD was developed by the Center for Naval Analyses (CNA). CONMOD resides on the IPS/TROLL system at the Massachusetts Institute of Technology.

2. Functional Capabilities: The TROLL system allows for direct user interaction with CONMOD. Simulation of any equation or the production of graphs is accomplished through simple conversation with TROLL. This system also provides for a variety of output options in addition to the printing of standard regression statistics. Econometric techniques ranging from OLS to 2SLS with autocorrelation correction procedures are readily available. CONMOD utilizes GLS because of the small sample sizes.

TROLL's unique file system allows all relevant files associated with a given model to be accessed automatically by referencing the model itself. The user doesn't need to be concerned with loading data or parameters. TROLL also contains a file editor and provides for off line printing.

3. Basic Assumptions: CONMOD was developed assuming the construction industry to be competitive. For any type of construction, the composition of construction between trades remains fixed.

Stock of structures equations imply a stock adjustment mechanism where actual stocks adjust to desired stocks at a constant rate (estimated by regression analysis). Lastly, the labor supply schedule is derived from a constant elasticity of substitution production function (CES).

4. Input and Output: Once CONMOD has been accessed, the TROLL system automatically provides the required data input. The user can then specify the equation technique, simulation period, required statistics, and any graphic output desired. After the model has been simulated once, TROLL will automatically create a 'data set' file which includes the model, data, and estimated coefficient values. In this way performing a variety of simulation experiments at a later time is a simple task. Data can be printed when desired and results from the output stream can be stored for later use.

5. System Resource Requirements: There are no specific system resource requirements needed to run CONMOD on TROLL. The system is conversational and costs approximately $9.00 per CPU minute and $2.00 per hour connect time to operate.

6. Applications: CONMOD is used for estimating the economic impact resulting from the EPA's massive sewer line and sewer treatment plant expenditure program. The model may also be used for other applications involving the construction industry.

7. Technical Contacts

James Titus
U.S. Environmental Protection Agency
Economic Analysis Division
PM-220
401 M Street, S.W.
Washington, D.C. 20460
COM 202/382-2774 FTS 382-2774

8. References

Center for Naval Analyses, March 1978. The Economic Effects of Environmental Regulations on the Construction Industry" Arlington, Virginia.

National Bureau of Economic Research, June 1972. "TROLL/1 Users Guide" Cambridge, Massachusetts.

SECTION 120 NONCOMPLIANCE PENALTY MODEL (PENALTY)

1. Model Overview: The Section 120 Noncompliance Penalty Model (PENALTY) is an economic model used to calculate the economic benefit of delayed compliance with the requirements of the Clean Air Act as amended, August 1977. The noncompliance penalty is based on the concept that it is usually in a source's best economic interest to delay the commitment of funds for pollution control equipment, and that incentive should be eliminated. The program was completed in February 1979, by Putnam, Hayes & Bartlett, Inc. of Newton, Massachusetts, for the U.S. EPA, Office of Planning and Management.

2. Functional Capabilities: PENALTY compares two cash flows: that which the source would have experienced had it achieved compliance on the date it received a notice of noncompliance, and that which it is estimated it will experience as a result of its delay. Because these cash flows occur at different times, a basis of comparison is provided by discounting them to their present value equivalents. The model then calculates the difference between these two cash flows and the appropriate quarterly payment schedule that the source should follow. It can also make a final adjusted penalty calculation when the source has achieved compliance. The capital investment portion of the penalty is calculated using standard and rapid amortization. Under both types of amortization, the program calculates the depreciation tax savings using straight line, sum-of-the-years-digits, and double declining balance depreciation methods. The program will automatically choose the method which will result in the lowest penalty.

3. Basic Assumptions: Assumptions of the penalty follow:

1) The relative mix of debt, preferred stock, and common equity allocated to pollution control equipment is the same as that found in the firm's capital structure as shown on its balance sheet.
2) Cash flows are discounted using the equity method.
3) The non-compliance penalty is computed as a non-tax deductible expense to the firm.
4) Cash flows take place at the end of each month.
5) The rate of inflation of pollution control operating and maintenance expenditures is the same as that for pollution control capital costs.
6) The noncompliance penalty is calculated using a thirty-year time horizon.
7) The salvage value of any equipment with useful life remaining at the end of the thirty year time horizon is zero.
8) The discount rate is not less than the inflation rate.

4. Input and Output: Input to the model includes source-related data: facility life, months of noncompliance income tax rate, discount rate, and preferred stock dividend rate; equipment-related data, capital expenditures, operating and maintenance costs, financing (industrial bonds; equity share, preferred stock share, and debt share of investment), equipment useful life and depreciation life; and a forecasted inflation rate. This information may come from the firm itself as well as the Internal Revenue Service, Chemical Engineering Plant Cost Inflation Index, the Federal Trade Commission, and Moody's Bond Record.

Output consists of two user-selected formats; a lump sum settlement, or a schedule of quarterly payments, both expressed in thousands of dollars.

5. System Resource Requirements: PENALTY is coded in FORTRAN. It is run on an IBM 360/370 mainframe. A background in economics and finance is helpful.

6. Applications: It is used by HQ and regional offices as well as sources and contractors to compute noncompliance penalties.

7. Technical Contact

Howard F. Wright
U.S. Environmental Protection Agency
Division of Stationary Source Enforcement
401 M Street, S.W.
Washington, D.C. 20460
COM 202/382-2833 FTS 382-2833

9. References

Federal Register. Monday, July 18, 1980. Part II - EPA - Assessment and collection of Non-Compliance Penalties by EPA and approval of State Non-Compliance Penalty Program.

Appendix A - Technical Support Document

Appendix B - CCA Section 120 Non-Compliance Penalties Instruction Manual

STEEL INDUSTRY MODEL (PTM)

1. Model Overview: PTM was developed by Temple, Barker, and Sloane (TBS) for the purpose of systematically analyzing the effects on the steel industry resulting from environmental regulations, input price changes, or from other cost variations. The model partially relies on a modeling effort previously done by Arthur D. Little in Cambridge, Massachusetts. PTM contains three modular components: production, pollution control, and finance. The two later components depend upon the production and capacity data from the production component in order to execute. Exogenous variable values for simulation were obtained through Chase Econometrics.

2. Functional Capabilities: PTM has the capability of performing many different sensitivity analyses by altering data inputs such as the rate of return on equity, degree of cost pass through, cost of capital, etc. In addition, effects on energy usage, employment, and the balance of trade stemming from environmental regulations can be estimated. Cost impacts of the Clean Air Act and other air pollution regulations can be calculated utilizing different engineering cost estimates. The resulting revenue requirements and price effects are also computed by the model.

3. Basic Assumptions: In establishing a baseline forecast for the steel industry, TBS has assumed that domestic steel shipments will rebound from 1975 recession levels. This adjustment is assumed to be completed by 1977 and, thereafter, steel shipments are assumed to follow the long run trend to 1983. The baseline forecast for steel shipments by 1980 is 120 million tons. The other baseline indicators needed to simulate the baseline forecast are capital expenditures, external financing needs, operations and

maintenance expenses, revenue requirements, and the average price of steel per ton. TBS has calculated the following numbers for the baseline forecast.

	Short Run 1975-1977	Long Run 1975-1983
Capital Expenditures	$ 8.7	$ 27.5
External Financing Needs	3.8	13.0
O&M Expenses	78.2	272.9
Revenue Requirements	96.1	338.6
Average Price (in 1975 dollars per ton)	345.26	365.21

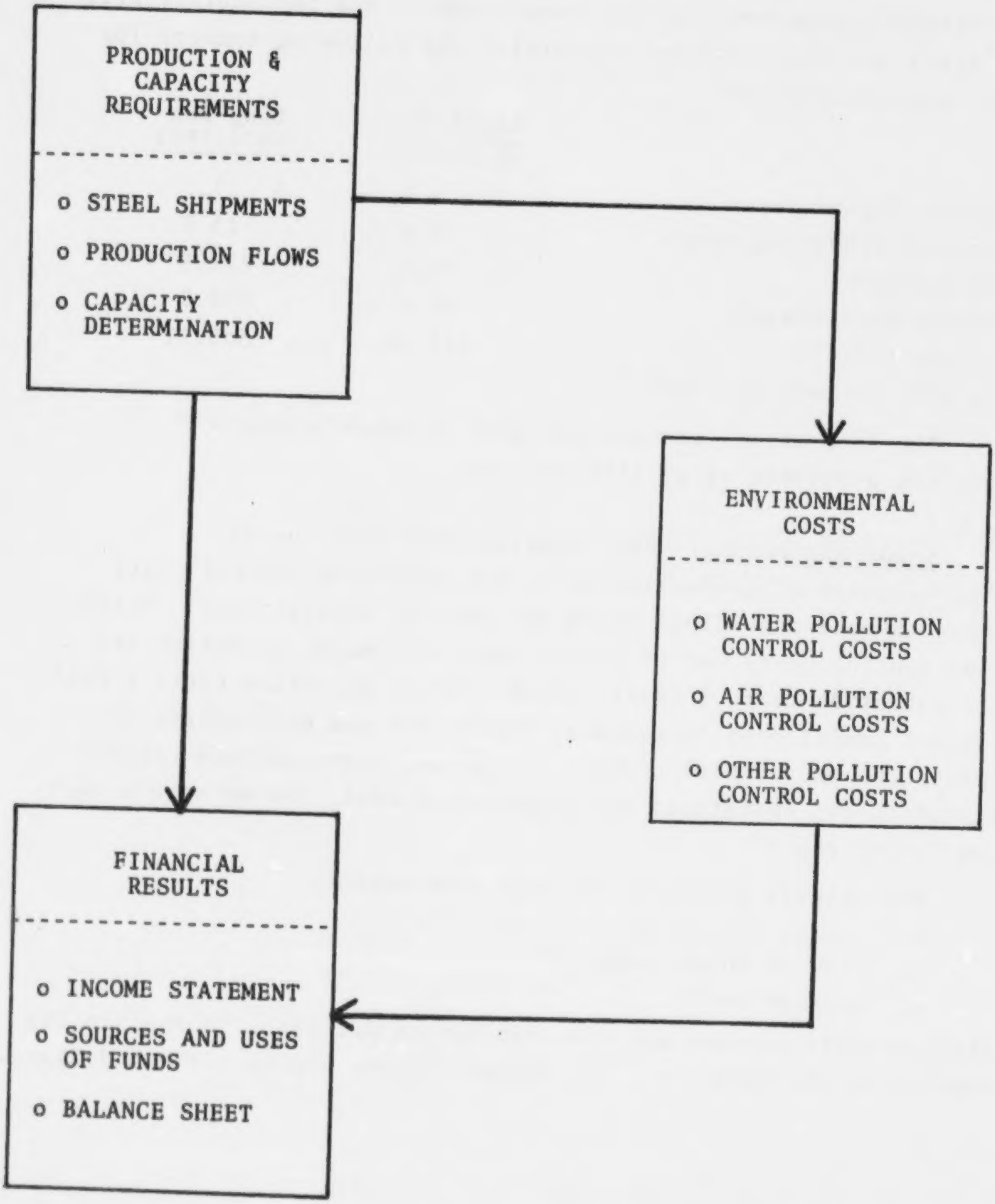
The theoretical assumptions used in constructing PTM were not available as of this writing.

4. Input and Output: PTM requires many cost inputs. These consist of production costs and pollution control costs. Under these two headings there are several subdivisions. Pollution control costs can be broken down into water pollution and air pollution control costs. Each type of pollution control cost has two (main) cost categories; operations and maintenance expenditures and capital costs. Production costs include capital expenditures, operations and maintenance cost, raw materials cost, and 'other costs'.

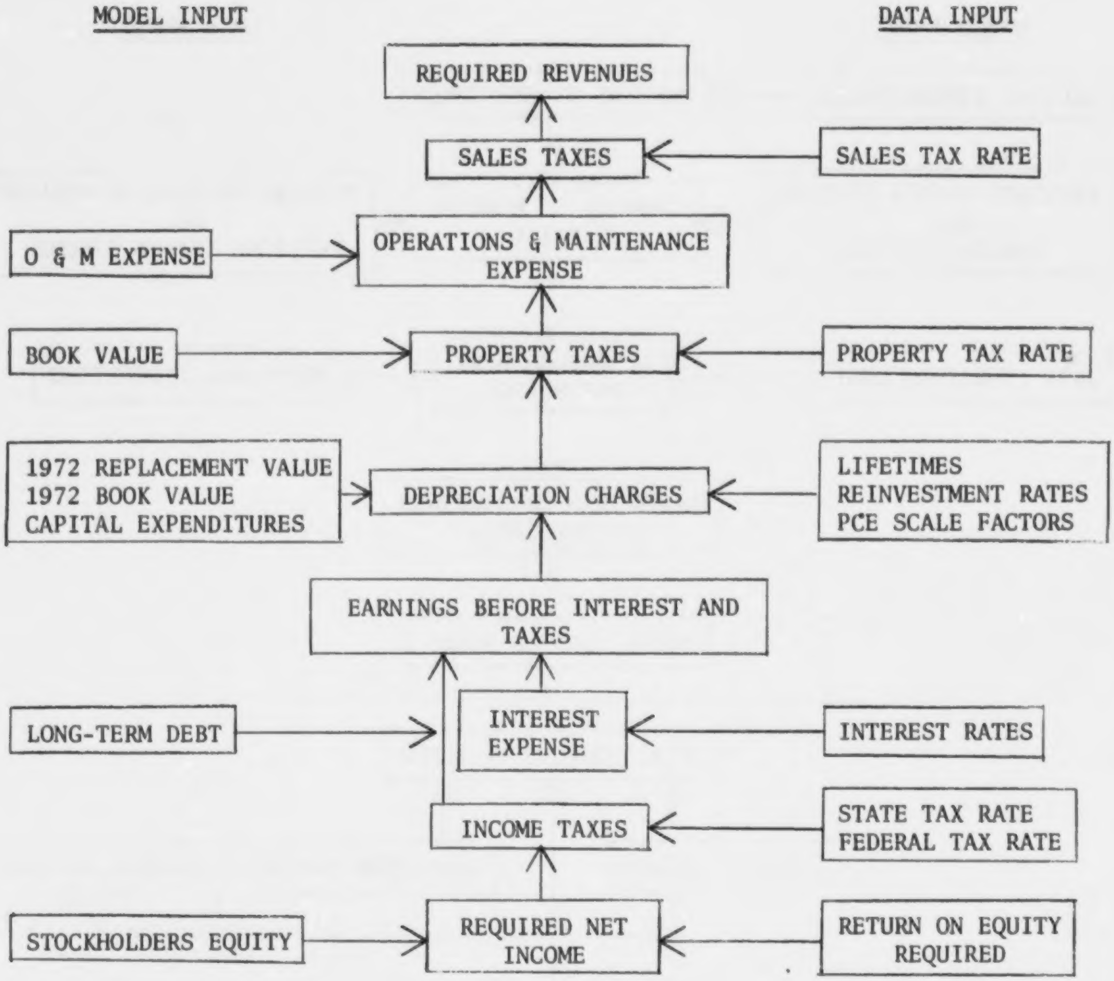
PTM (Steel) produces the following outputs:

1. Income Statement
2. Flow of funds summary
3. Balance sheet

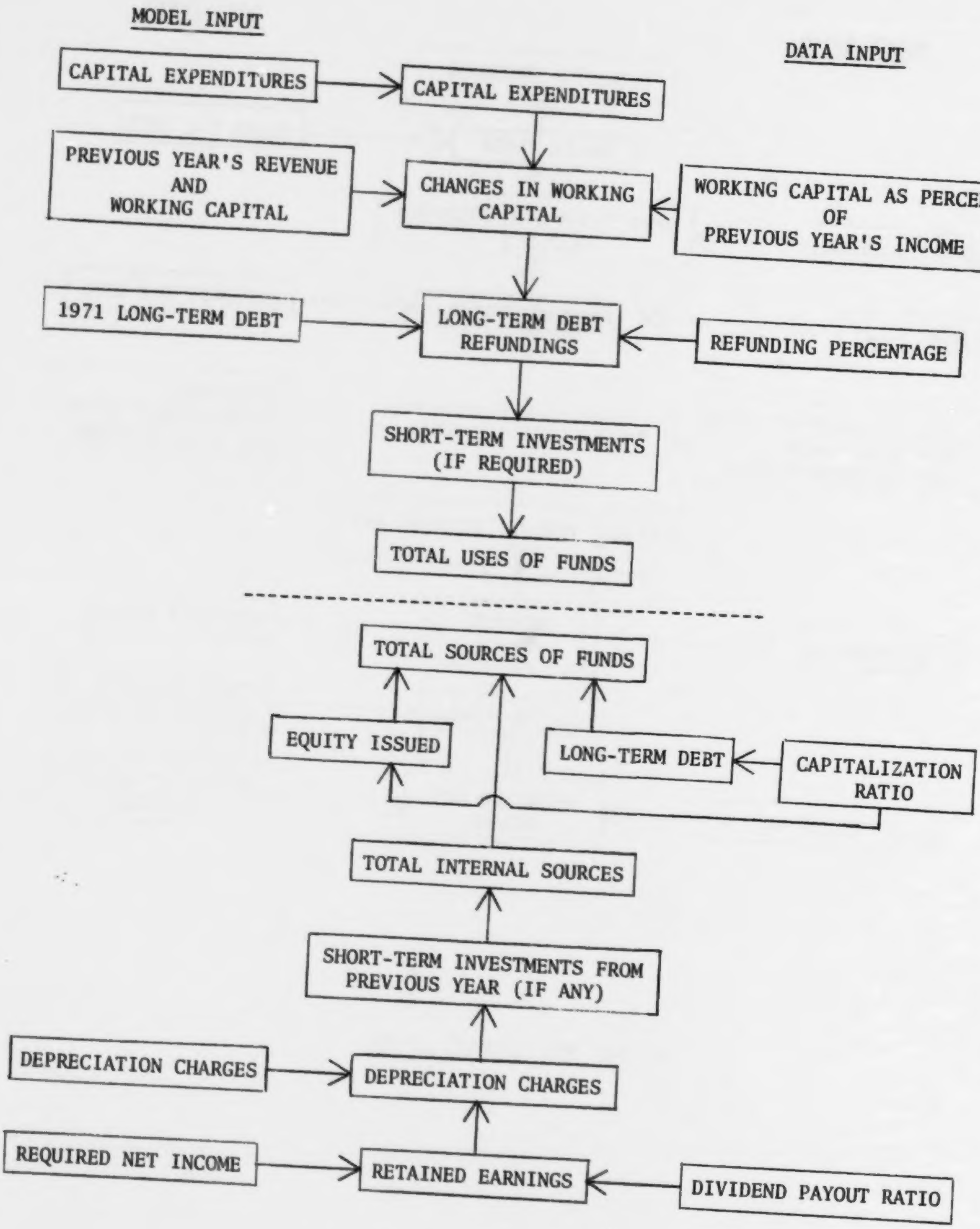
These outputs contain all the information necessary to analyze the impacts on the industry. All output figures are in current dollars.


PRODUCTION & CAPACITY REQUIREMENTS
o STEEL SHIPMENTS
o PRODUCTION FLOWS
o CAPACITY DETERMINATION
ENVIRONMENTAL COSTS
o WATER POLLUTION CONTROL COSTS
o AIR POLLUTION CONTROL COSTS
o OTHER POLLUTION CONTROL COSTS
FINANCIAL RESULTS
o INCOME STATEMENT
o SOURCES AND USES OF FUNDS
o BALANCE SHEET

PTM MAJOR COMPONENTS


MODEL INPUT
DATA INPUT
REQUIRED REVENUES
SALES TAXES
SALES TAX RATE
O & M EXPENSE
OPERATIONS & MAINTENANCE EXPENSE
BOOK VALUE
PROPERTY TAXES
PROPERTY TAX RATE
1972 REPLACEMENT VALUE
1972 BOOK VALUE
CAPITAL EXPENDITURES
DEPRECIATION CHARGES
LIFETIMES
REINVESTMENT RATES
PCE SCALE FACTORS
EARNINGS BEFORE INTEREST AND TAXES
LONG-TERM DEBT
INTEREST EXPENSE
INTEREST RATES
INCOME TAXES
STATE TAX RATE
FEDERAL TAX RATE
STOCKHOLDERS EQUITY
REQUIRED NET INCOME
RETURN ON EQUITY REQUIRED

INCOME STATEMENT LOGIC


MODEL INPUT
DATA INPUT
CAPITAL EXPENDITURES
CAPITAL EXPENDITURES
PREVIOUS YEAR'S REVENUE AND WORKING CAPITAL
CHANGES IN WORKING CAPITAL
WORKING CAPITAL AS PERCENT OF PREVIOUS YEAR'S INCOME
1971 LONG-TERM DEBT
LONG-TERM DEBT REFUNDINGS
REFUNDING PERCENTAGE
SHORT-TERM INVESTMENTS (IF REQUIRED)
TOTAL USES OF FUNDS
TOTAL SOURCES OF FUNDS
EQUITY ISSUED
LONG-TERM DEBT
CAPITALIZATION RATIO
TOTAL INTERNAL SOURCES
SHORT-TERM INVESTMENTS FROM PREVIOUS YEAR (IF ANY)
DEPRECIATION CHARGES
DEPRECIATION CHARGES
REQUIRED NET INCOME
RETAINED EARNINGS
DIVIDEND PAYOUT RATIO

FLOW OF FUNDS LOGIC

5. System Resource Requirements: PTM is coded in FORTRAN V and can be run on the IBM 370/158 or Univac 1110 computers. Unless alterations to the baseline or scenario forecasts are desired, the model can be run immediately after being loaded into the machine. Direct alterations to the program would require a working knowledge of FORTRAN and econometrics.

6. Applications: PTM Steel has been primarily used for environmental impact/sensitivity analyses by the U.S. Environmental Protection Agency. The model could also be used in forecasting impacts on the steel industry resulting from changes in factors of production, factor prices, or technological advancement.

7. Technical Contacts

Robert Greene
U.S. Environmental Protection Agency
Economic Analysis Division
PM-220
401 M. Street, S.W.
Washington, D.C. 20460
COM 202/382-5480 FTS 382-5480

8. References

Temple, Barker, and Sloane (TBS) July 1977. "Analysis of Economic Effects of Environmental Regulation on the Integrated Iron and Steel Industry" Volumes 1 and 2. Wellesley Hills, Massachusetts.

STRATEGIC ENVIRONMENTAL ASSESSMENT SYSTEM (SEAS)

1. Model Overview: The Strategic Environmental Assessment System (SEAS) is a comprehensive forecasting system which can be used to determine the environmental, economic, and energy effects of differing growth patterns and policies. Depending upon its use, the forecast horizon for SEAS can be from one to fifty years, with the range of 15-25 years for the most common projections. The SEAS model was developed at EPA and operating versions are in existence at EPA.

2. Functional Capabilities: The SEAS system is modular in nature in that any program may be executed independently of the others provided that all mandatory input files have been created previously. Each program produces a detailed printed output report and an output file for processing by other programs. In addition, general purpose report generators are available for the production of system summary reports.

All programs are autonomous in the sense that they do not require mandatory user-supplied information. A "default scenario" run reflects forecasts based on the best data available from government sources, excluding any external input information. Each SEAS program will accept two types of user-supplied information:

1) Execution Options. The selection of years to be processed is an option common to all programs except INFORUM. In addition, optional scenario conditions may be applied to all programs. Each scenario corresponds to a certain set of parameter values and conditions. By selecting a given scenario, these data values are automatically set by the program.
2) Override of Default Data. The user must specify each item of the substitute data.

The SEAS programs may be grouped and categorized according to functional capability. Each functional unit of the SEAS system is referred to in this report as a "module". The following is a description of most of the modules in the system:

1) INFORUM: An expanded version of the University of Maryland's INFORUM interindustry input-output model, which may be driven by alternate national macroeconomic forecasts.
2) Sector Disaggregation (INSIDE): Disaggregation of INFORUM economic sectors to represent subsector growth and technological change in greater detail.
3) Abatement Costs (ABATE): Capitol costs, and operating and maintenance (O&M) costs associated with the control of pollution for each economic sector and subsector.
4) Relative Commodity Prices: Adjusts industrial forecasts to account for the impact on relative prices due to pollution control activity or stock shortage.
5) Stock Reserves and Prices (STOCKS): Accounts on domestic and worldwide reserves of critical resources and materials as determined by relative production price, investment requirements, and net import levels.
6) Solid Waste/Recycle (SOLRECYC): Annual tonnage, disposal methods, and costs for non-industrial and solid waste sources, and estimated levels of recycling.
7) National Residuals (RESGEN): Estimates of annual tonnage of air, water, and land pollution from stationary sources on a nation-wide basis.
8) The Energy Demand Modules (Residential/Commercial, Industrial, Transportation): Calculates the energy demand due to activities in these sectors. The level of activity for each of the sectors depends on the economic scenario currently being utilized.
9) Energy System Network Simulator (ESNS): An adaptation of the ESNS network was developed at Brookhaven National Laboratories. For each set of energy demands the network traces end use through the processes of extraction, transportation and conversion. Residuals produced during these processes are calculated in ESNS.
10) Regionalization (REGION): Regionalization of national economic, pollutant, and abatement cost data.

11) Land Use: Forecasts of urban, rural and agricultural land use and associated nonpoint residuals.

12) Ambients (AIRAMB, WATERQUAL): Surrogate measures of ambient air and water effluent discharge levels (experimental).

A module flowchart illustrating the standard module configuration is presented. A brief explanation of the flow of information is given in the following narrative.

National economic forecasts are generated by a common program consisting of INFORUM, Sector Disaggregation, and Abatement Cost modules. Economic output forecasts from INFORUM are first input to Sector Disaggregation for more detailed industrial forecasts. The Sector Disaggregation may require feedback from INFORUM to adjust the output forecasts of certain related sectors. Sector growth rates, at the disaggregated level, are then used in the computation of abatement cost estimates for predefined control technologies within each sector. Internal feedbacks from these computations automatically adjust the coefficients in the various matrices in INFORUM. The integrated economic model iterates through this solution procedure twice for each forecast year. (The user, however, may at his option, shut off either the Abatement Cost module or the Sector Disaggregation module, or both.)

Nationwide solid waste residuals and recycling levels are calculated in the Solid Waste/Recycling module. Levels of depletable resources are calculated from consumption levels and recycling levels. Residential/commercial, industrial, and transportation energy demands are calculated in the demand modules based upon the national economic forecasts. The Energy System Network Simulator calculates the amounts of extraction, transportation and conversion necessary to meet the energy demands. Both the Transportation Energy Demand module and the ESNS calculate residuals resulting from their activity levels.

Residuals and economic abatement costs forecasts are regionalized to various regional classification schemes in the Regionalization module. Regional transportation emissions, computed within the transportation module, may be added to the regional residuals data file. Regional land use activity, residuals, and ambient pollutant concentrations can also be calculated.

The levels of resources and materials cause changes in prices. Significant changes in prices may necessitate feedback to INFORUM to adjust the national economic forecasts.

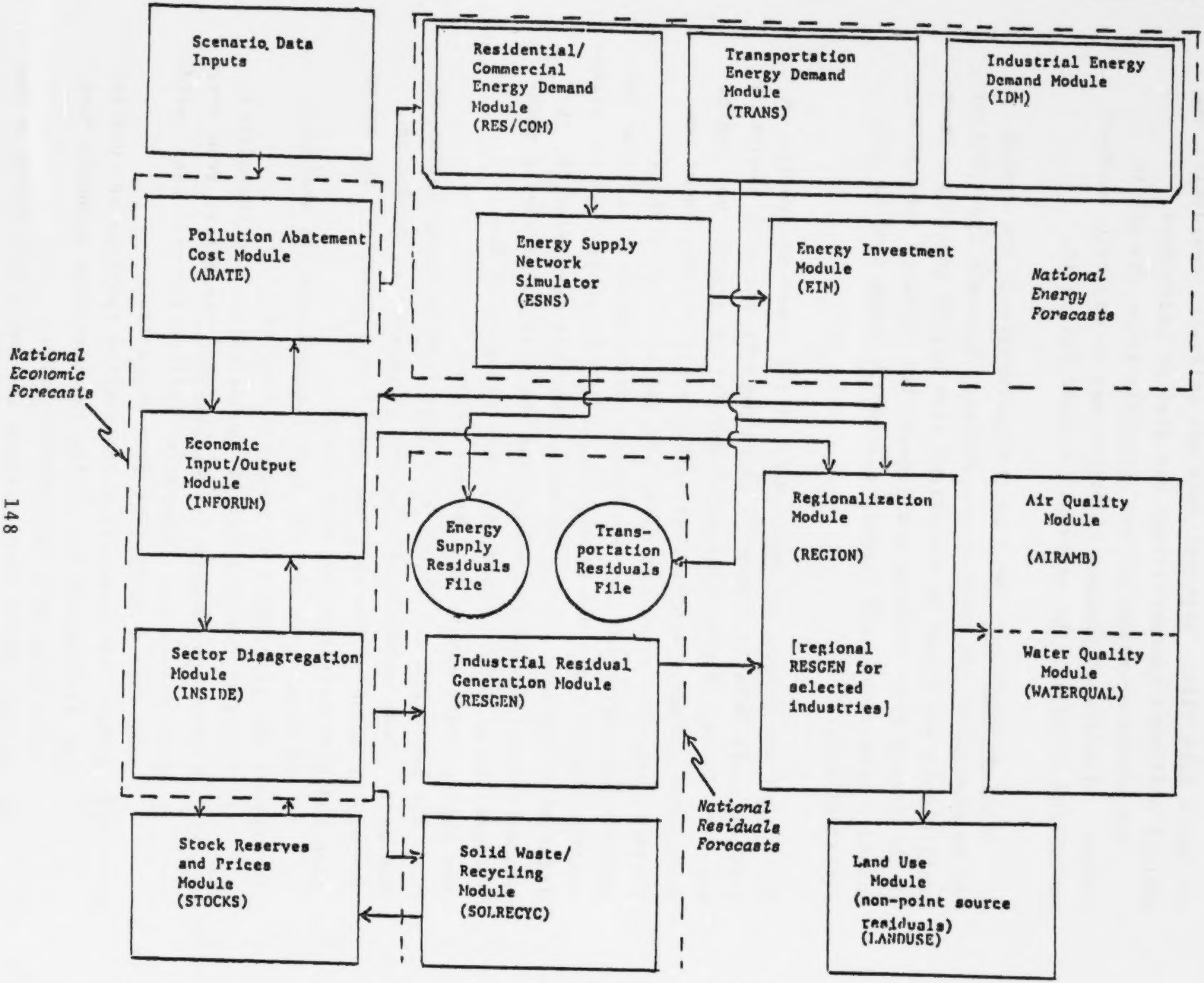
3. Basic Assumptions: Most of the parameters in the system can be changed by the user of the system. Economic input/output coefficients are based on historical time series analysis. Most of the direct relationships are linear, but resource constraints, boundary conditions, and iterative feedback loops produce non-linear effects.

4. Input and Output Options: Many of the input parameters in SEAS exist as default values to be changed by the user should he elect to do so. Assumptions about population growth, per capita disposable income, unemployment rates, years for abatement compliance, price of gasoline, miles per gallon fleet mixes for automobiles, logistics for new technological process mixes in industry, changing product mixes, increasing or shortening the viable lifetime of durable goods, the recycling rate for industry, the composition of demand for energy, and the mixture of supply technologies to meet the demand, are some examples of the types of input changes that can be made to the system.

The selection and format of output reports is an option of the user. Each module in the system is capable of producing a variety of outputs; the user may specify the points in the execution and categorization of that output.

In addition, four general report generators are available to support the assessment of scenario results:

1) POSTCOMP, which provides annual values and annualized percentage changes for significant parameters from every SEAS module and comparative indices for pollutant residuals from a maximum of four scenarios.
2) INFRPT, which provides comparative rankings and percentage differences for sector and subsector economic forecasts from selected scenario pairs.
3) RANKER, which ranks sectors and subsectors based on the


Scenario Data Inputs
Residential/ Commercial Energy Demand Module (RES/COM)
Transportation Energy Demand Module (TRANS)
Industrial Energy Demand Module (IDM)
Pollution Abatement Cost Module (ABATE)
Energy Supply Network Simulator (ESNS)
Energy Investment Module (EIM)
National Energy Forecasts
National Economic Forecasts
Economic Input/Output Module (INFORUM)
Energy Supply Residuals File
Trans-portation Residuals File
Regionalization Module (REGION)
[regional RESGEN for selected industries]
Air Quality Module (AIRAMB)
Water Quality Module (WATERQUAL)
Sector Disagregation Module (INSIDE)
Industrial Residual Generation Module (RESGEN)
National Residuals Forecasts
Stock Reserves and Prices Module (STOCKS)
Solid Waste/ Recycling Module (SOLRECYC)
Land Use Module (non-point source residuals) (LANDUSE)

SEAS System Flowchart

annual amount of net residuals for each pollutant in a specified medium, at either national or regional levels.

4) CLEANSUM, which provides annual pollution control costs and residuals associated with predefined processes and abatement technologies.

5. System Resources Requirements: Most of the SEAS module algorithms are written in FORTRAN IV-G1, and the system is installed on an IBM 370/158 computer. The programs do not require any special software packages and are available on both OS and VS IBM operating systems. SEAS modules require from 70K to 650K bytes of main storage depending upon the modules being run, and most modules require 250K of storage or less.

6. Applications: The Strategic Environmental Assessment System has been used for both comprehensive and issue-specific applications within EPA and within other public and private institutions and government agencies. Within EPA, SEAS has been used to support several ORD Integrated Technology Assessment (ITA) projects including the Western Energy Development ITA and the Ohio River Basin Energy Study ITA. SEAS is also used to provide environmental trends projections to support the production of ORD's annual Research Outlook. SEAS was also used within EPA to produce the 1976 Cost of Clean Air and Cost of Clean Water reports.

The Department of Energy (DOE) uses SEAS to analyze the implications of alternative patterns of energy and economic development in the National Environmental Impact Projection Series (NEIP). DOE also uses SEAS to support internal planning and budgeting activities and to produce the Annual Environmental Analysis Report. In addition SEAS forms a major part of the DOE Transportation Energy Conservation Network (TECNET), which forecasts impacts of transportation energy conservation initiatives.

Resources for the future has used SEAS to forecast implications of population growth through the year 2025. The Solar Energy Research Institute has used SEAS to forecast the environmental and economic implications of alternative penetrations of solar technologies. There are and have been numerous additional applications of the system.

7. Technical Contacts:

John J. Coleman
U.S. Environmental Protection Agency
Office of Research and Development
401 M St. S.W.
Washington, D.C. 20460
COM 202/382-2608 FTS 382-2608

Basil Manns
U.S. Environmental Protection Agency
Office of Research and Development
401 M St. S.W.
Washington, D.C. 20460
COM 202/245-3026 FTS 245-3026

8. References

House, P.W. Trading-off Environment, Economics, and Energy: A Case Study of EPA's Strategic Environmental Assessment System. Lexington, Massachusetts: D.C. Heath & Company, 1977.

Control Data Corporation. AEAR/TAMP User's Guides. 2 vols. Prepared for the Department of Energy, Washington, D.C., by Control Data Corporation, Rockville,MD , November 1977.

Control Data Corporation. AEAR/TAMP Data Specifications. Prepared for the Department of Energy, Washington, D.C., by Control Data Corporation, Rockville, MD , November 1977.

Control Data Corporation. AEAR/TAMP Program Specifications. 2 vols. Prepared for the Department of Energy, Washington, D.C., by Control Data Corporation, Rockville, MD , November 1977.

U.S. COPPER INDUSTRY MODEL (COPMOD1)

1. Model Overview. The financial-econometric simulation model of the U.S. Copper Industry has been developed to assess the industry-wide economic impact of compliance with the air and water pollution abatement legislation. The model consists of a market clearing module and a dynamic investment module programmed in FORTRAN. COPMOD1 was constructed by Arthur D. Little, Cambridge, Massachusetts.

2. Functional Capabilities. COPMOD1 incorporates two versions of the U.S. Copper model, linear and nonlinear. The model identifies three alternative modes of pricing behavior for the primary producers in the linear and nonlinear cases:

1. Price = Average Variable Cost	(slack demand)
2. Price = Average Total Cost	(normal demand)
3. Marginal Revenue = Marginal Cost	(demand 'crunch')

The nonlinear version permits the introduction of capacity constraints in supply and cost curves, whereas the linear version yields unconstrained production estimates. Plant capacity could be exceeded in the linear simulation experiment.

In addition, subroutines are included to plot average total cost, average variable cost, average fixed cost,and compare historical period simulation results with actual data.

3. Basic Assumptions. The model explicitly assumes the following market classifications:

1. Primary producers
2. Secondary refiners
3. Producers of non-refined scrap

These classifications are based upon pricing behavior and production technology. More importantly, primary producers are analyzed as behaving oligopolistically while secondary refiners and producers of non-refined scrap are treated as behaving competitively.

4. Input and Output. Alteration of the scenario file in COPMOD1 can take two forms:

1. Card input
2. File editor

Due to the structure of the program, modification of the scenario file is most easily accomplished using the file editor. Modification through card input can only occur if the entire program subroutine with the new cards is reloaded into the computer. As of this writing, program modification remains non-interactive.

COPMOD1 provides for the following input options:

1. Specification of model version:
    a. Linear
    b. Nonlinear
    c. Both
2. Printing of all endogenous and exogenous variables.
3. Printing of various diagnostic variables.
4. Which of the three parametric solutions (P = ATC, P = AVC, MR = MC) is most probable.

Depending upon the version chosen, COPMOD1 will generate a wide range of subsidiary calculations such as production estimates, sales estimates, and payroll estimates. Financial estimates (pollution abatement investment, depreciation, dividends, etc.) derived from primary producer's estimated fixed costs are printed in constant and current dollars.

5. System Resource Requirements. COPMOD1 is coded in (ASCII) FORTRAN V and requires approximately 65K words of core storage for execution. The program is compatible with the Univac 1110 and a moderate amount of computer skills and a working knowledge of econometrics is useful.

6. Applications: COPMOD1 was developed primarily for estimating the impact on copper producer's costs from pollution abatement expenditure. The model may also be utilized in evaluating the effects of noncompliance fees on the producers of copper and non-refined scrap.

Technical Contacts

7. James Titus
U.S. Environmental Protection Agency
Economic Analysis Division
PM-220
401 M Street, S.W.
Washington, D.C. 20460
COM 202/382-2774 FTS 382-2774

8. References

Arthur D. Little, October 1976. "Economic Impact of Environmental Regulation on the U.S. Copper Industry". Draft report.

Arthur D. Little, April 1978. "COPMOD1 Program, Documentation", Cambridge, Massachusetts.

Raymond S. Hartman, January 1977. "An Oligopolistic Model of the U.S. Copper Industry" Ph.D thesis, M.I.T.

CONSTRUCTION SITE HEALTH AND WELFARE MODEL (CSM)

1. Model Overview: The model computes noise impacts on the population surrounding more than two million construction sites that are active every year in the U.S. In addition, the model computes the relief accruing to the various populations affected by construction site noise as a result of individual and combined regulations for one or more of the operational types of equipment.

2. Functional Capabilities: The complete model contains the following:

1) Time stream

2) Curve

3) Output of impact reduction

4) Distribution of Level Weighted Population (LWP) and population exposed with respect to 1 decible (1 db) level of noise day-night average (Ldn) intervals

5) Usage factors

6) Duration of construction site activity

7) Daytime population density shifts

3. Basic Assumptions: There are no basic assumptions.

4. Input and Output: Inputs to the CSM are:

1) Noise levels of construction equipment

2) Equipment usage factors

3) Number of construction sites by the type of site and by population density category

4) Population density

5) Duration of construction activity by phase of construction

Outputs to the CSM are:

1) Yearly Ldn

2) Equivalent sound level

3) Population exposed

4) Level Weighted Population (LWP)

5) Sound propagation distance to criteria levels

6) Relative change in impact

5. System Resource Requirements: CSM is coded in FORTRAN and is run on an IBM 370/168 mainframe. It uses any 132 position printer. Manpower needs include a background in engineering.

6. Applications: No outside use is allowed unless designated by Office of Noise Abatement and Control.

7. Technical Contact

Ken Feith
U.S. Environmental Protection Agency
Office of Noise Abatement and Control
Crystal Mall #2, Room 1101
1921 Jefferson Davis Highway
Arlington, VA 22202
COM 703/557-2710 FTS 557-2710

8. References

No references are available.

NATIONAL ROADWAY TRAFFIC NOISE EXPOSURE MODEL

1. Model Overview: The model deterministically estimates extent and severity of noise exposure in the U.S. due to motor vehicles operating on the national roadway network. The model is used primarily for assessing the national impact of various noise control strategies, including source control. The structure of the model is based on extensive roadway data, demographic data, and vehicle use and noise data. Time series projections are also calculated on all time dependent variables where data are available.

2. Functional Capabilties: The accuracy of the model is indeterminate since the basic output is noise impacts on a national scale.

3. Basic Assumptions: The model is based on the equivalent sound level methodology and calculates various impact metrics. The model calculates general adverse response impacts (energy summation) as well as single event impact (independent sources assumption). Propagation losses are on the usual excess attenuation approach with values assigned by site type. Site types are hard, soft, or built up urban site types.

4. Input and Output: Inputs are vehicle, roadway, and population data; years for scenario; vehicle noise levels by vehicle type, speed, and mode of driving; population projection; and vehicle fleet forecast.

Outputs of the model are plots of exposure contours, health and welfare metrics for general adverse responses, single event responses. Health and welfare metrics include number of level-weighted people, relative exposure in percent, noise impact index, number of people exposed by area and roadway type in dB bands, LWP by roadway type, and area type in dB bands per year of time-stream.

5. System Resource Requirements: The model is written in FORTRAN IV. It is run on an IBM 370 mainframe. Operation requires a computer programming background.

6. Applications: This model was used for the health and welfare analyses to examine the effectiveness of selected noise regulatory options.

7. Technical Contact

Fred Mintz
U.S. Environmental Protection Agency
Standards and Regulations Division
Crystal Mall #2, Room 1105
1921 Jefferson Davis Highway
Arlington, VA 22202
703/557-2710

8. References

Model documentation is being prepared.

RAILROAD HEALTH AND WELFARE MODEL (RMEA 79N3)

1. Model Overview: The model estimates national noise exposure due to railroad operations. It calculates the noise emissions from individual railyard operations of selected yards. These railyards are selected statistically to represent the national distribution of railyard type and classification. The noise levels are calculated at the boundary of the railyards and propagated into occupied land use areas. Thus, the results are noise exposures due to railyard operations. From the statistically defined sample of railyards, the resultant exposures are extrapolated to the national level by yard types and then summed.

2. Functional Capabilities: The model calculates the present exposure due to railyard operations. It can be used to calculate the total exposure from one railyard to any number of railyards, knowing the basic characteristics, size, type, and activity level of the railyard. The population distribution around the yard must also be known.

3. Basic Assumptions: Refer to "Description of Railroad Health and Welfare Model" for basic assumptions of the model.

4. Input and Output: Input to the model consists of:

1) Engine noise from locomotives and switch engines
2) Retarder squeal noise
3) Refrigerator car noise
4) Car-coupling noise
5) Load cell testing, repair facilities and locomotive service area noise
6) Wheel/rail noise
7) Horns and address systems
8) Regulatory scenarios

The output consists of exposure descriptors for any aggregated set of railyards, total LWP, benefits due to a regulatory schedule, and the number of people actually exposed to various levels of noise.

5. System Resource Requirements: RMEA 79N3 is coded in FORTRAN and is run on an IBM 370.

6. Applications: The model has been used for internal EPA-Office of Noise Abatement and Control decision-making purposes.

7. Technical Contact

Basil H. Manns
U.S. EPA
Office of Research and Development
401 M Street, S.W.
Washington, D.C. 20460
COM 202/245-3026 FTS 245-3026

8. References

1. Description of Railroad Health and Welfare Model
2. User's Manual for the Railroad Health and Welfare Model
3. Programmer's Manual for the Railroad Health and Welfare Model

A MATHEMATICAL MODEL FOR FAST-SCREENING PROCEDURE FOR TESTING THE EFFECTS OF POLLUTANTS IN MAMMALS

1. Model Overview: The model offers an "on-line" method for measuring the effect of pollutants on respiratory efficiency in mammals, and it applies to any biological system in which the transport of matter is through well-defined compartments.

Since CO_2 excretion from the lungs (a measure of efficiency of respiratory function) has a well-defined distribution with time, it can be used for the prediction of effects by pollutants entering the body system. In this particular case, the model was derived for the prediction of the effect of ingested methylmercury chloride (11) on the excretion of $^{14}CO_2$ from the lungs. This method reduces the observation period from several hours to only a few minutes.

It is suggested that this model or a similar one can be used for measuring the efficiency of other body functions, provided that there exists a measurable parameter that has a well-defined distribution with time.

2. Functional Capabilities: The model is in the form of a fourth order differential equation requiring a solution of eight equations. Using mathematical methods of approximation, the model can be fitted precisely to a two-parameter model of the form: $R = B_1 t \exp(-B_2 t)$, where $\dot{R}$ is the rate of excretion of $^{14}CO_2$. In this form, only two measurements at the beginning of the experiment are required in order to predict the effects of the pollutant on respiratory function.

The measure of effects is the difference of cumulated $^{14}CO_2$ excreted $[R\ (+) = \int_o^t \dot{R}\ dt]$ between the control animals and the exposed animals.

3. Basic Assumptions: It is assumed that a two-pool open system exists (Shipley and Clark, 1972) in which the blood pool is the central compartment while the second pool is a conglomerate of peripherals such as the kidneys, lungs, and liver. Peripheral pools can communicate only through the central compartment. If we ignore the dead space in the respiratory tract, then the lung can be considered as composed of two classical compartments (Riley, 1965): the gas-exchange compartment, and the anatomical dead space in the alveoli. The model is based on the fact that the blood is the vehicle by which the effect of an ingested toxicant, such as CH_3HgCl, is superimposed on all other peripherals, thus influencing the $^{14}CO_2$ pattern. Each component is assumed to follow first-order kinetics in that the $^{14}CO_2$ loss rate is taken to be proportional to the number of moles of the $^{14}CO_2$ within a compartment. Actually, excretion from the blood pool is not linear (Piotrowski, 1971). But, as we assume, when steady-state kinetics apply, the blood pool can also be treated as a classical compartment (Aris, 1966).

4. Input and O[illegible] [illegible]del requires only two measurments of $^{14}CO_2$ from C[illegible] reed electrometers in conjuction with [illegible] chambers. Output of the model is the total cumulative value of ^{14}C excreted and the percent of ^{14}C excreted.

5. System Resource Requirements: Solutions to the model can be obtained on a DEC 10 computer, but the model is simple enough that it can be solved on any other computer system or calculator.

6. Applications: The model has been used for a series of experiments by the Health Effects Research Laboratory of the EPA, and it can be used in biological investigations where there is a need for a fast screening of pollutants (e.g., heavy metals or chemical compounds). The effects on respiratory efficiency or cardiac output can be predicted in a short time, thus saving time, animals, and personnel. This same approach can be developed from any other body function with a well defined time distribution via a compartmental analysis.

7. Technical Contacts

Rumult Iltis and Robert L. Miller
U.S. Environmental Protection Agency
Health Effects Research Laboratory
26 W. St. Clair Street
Cincinnati, OH 45268
FTS 684-7417 COM 513/684-7417

8. References

Iltis, R. and Miller, R.L. "A Fast-Screening Procedure for Testing the Effects of Pollutants in Mammals." *Journal of Toxicology and Environmental Health*, 3:683-689, 1977.

Itis, R. "Mathematical Model for the Excretion of $^{14}CO_2$ During Radio Respirometric Studies." *Proceedings of the Conference on Environmental Modeling and Simulation*. U.S. EPA publication EPA 600/9-76-016, July 1976.

Aris, R. Compartmental Analysis and the Theory of Residence Time Distribution in Intercellular Transport, ed. K.B. Warren. New York: Academic Progess, 1966.

Piotrowski, J. The Application of Metabolic and Excretion Kinetics to Problems of Industrial Technnology. Washington, D.C.: Department of Health, Education, and Welfare, 1971.

Riely, R.L. "Gas Exchange Transporation," Physiology and Biophysics, eds. T.C. Ruch and H.D. Patton. London: Saunders, 1965.

Shipley, R.A. and Clark, R.E. Tracer Methods for in Vivo Kinetics. New York: Academic Press, 1972.

PREMIXED ONE-DIMENSIONAL FLAME CODE (PROF)

1. Model Overview: The PROF code can be used to predict the detailed chemical kinetic combustion and/or pollutant formation events which occur in a wide variety of experimental and practical combustion devices. Both steady, free and confined premixed flames, where gaseous diffusion is important, can be treated by the code. Also, well-stirred reactor, plug-flow reactor, and fixed mass time-evolution chemical kinetic problems, where diffusion is not explicitly treated, can be modeled by the code. The code was completed in February 1978 by the Acurex Corporation/Energy & Environmental Division of Mountain View, California. (Previously called: Modeling Studies in Combustion Aerodynamics/Chemistry.)

2. Functional Capabilities: The PROF code was developed to accurately model the detailed combustion and pollutant formation processes occurring in premixed one-dimensional flames. Previous plug-flow models applied to premixed flame combustion and pollutant formation processes did not incorporate axial diffusion in the formulation. Since ignition processes require upstream diffusion, these plug-flow models could not be directly applied to flames without making some gross assumptions as to the upstream ignition zone starting conditions. In addition, the accuracy of these nondiffusive models is very poor in the flame zone, where diffusion is important. Since the PROF code includes axial diffusion, predictions of combustion and pollutant formation processes can be achieved in the flame zone as well as downstream of this zone. The accuracy of these predictions is dependent only on the adequacy of elementary kinetic reaction and transport data. Thus, PROF predictions, combined with experimental data, can provide valuable insights into the complex chemical events taking place within and downstream of the flame zone.

3. Basic Assumptions: The key program element in the PROF code is a stable and reliable kinetic chemistry routine. This routine can be applied to any chemical system for which kinetic reaction data are available. Flame and reactor-type problems are modeled by linking appropriate drive routines to the general chemistry routine. The flame model includes axial gas phase diffusion and is, mathematically, a multivariable boundary value problem. This problem requires a coupled grid solution procedure for all variables. This grid problem is solved in PROF by using a predictor-linearized corrector iterative matrix procedure. The reactor type models do not have explicit diffusion terms. These models are initial value problems solved by simple time or space matching in the PROF code.

4. Input and Output: Input to the code include: solution type (e.g., well-stirred reactor), names and number of chemical species, thermochemical data for chemical species, chemical reactions and associated forward rate constants, third body efficiencies, initial mole fractions, temperature, pressure, and flow rates.

The PROF code output gives complete summary information or flame, well-stirred and plug-flow reactor, and time-evolution chemical kinetic problems. If called for, it can also provide information on intermediate iterations and chemistry routine solutions. For each iteration during a flame solution the code always prints out a line of output that gives the flame speed parameters, its error, the maximum error in concentration, and the constraint (i.e., damping) applied to the corrector step correction vector. In addition, all of the input data is output along with the title of the run.

5. System Resource Requirements: The PROF is written in FORTRAN and can be run on an Univac 1108, IBM 360 or CDC 6600

mainframes. Disk storage requirements include 15,355 words of decimal storage for the model and 31,978 words of decimal storage for data. Additional and peripheral equipment required includes magnetic tape or disk storage, a 132 line printer and a card reader/punch or tape/disk (input).

6. Applications: The PROF code has been used widely by Acurex and the Environmental Protection Agency to predict the pollutant formations that occur in a wide variety of experimental and practical combustion devices. The code has been applied to a variety of gas turbine, furnace and catalytic combustion, and pollutant formation problems. The PROF code has also been used to treat the reaction of a fixed mass of gas in time as the pressure and temperature change. Chemical evolution inside internal combustion engines, combustion bombs, and other time-dependent combustion systems have been predicted by this option. Of course, the option assumes uniformly mixed and reacting mixtures within the system. Therefore, applying this option to spatially non-uniform systems represents only an approximation modeling of the system.

7. Technical Contact

W. Steve Lanier
U.S. Environmental Protection Agency
Industrial Environmental Research Laboratory
Research Triangle Park, N.C. 27711
COM 919/541-2432 FTS 629-2432

8. References

Kendall, R.M. and Kelly, J.T. Premixed One-Dimensional Flame (PROF) Code User's Manual, EPA-600/7-78-172a, August 1978.

WASTE RESOURCES ALLOCATION PROGRAM (WRAP)

1. Model Overview: WRAP is a waste resources allocation program which is coded in FORTRAN. This modeling program consists of a series of equations which consider the sources of solid waste generation, a set of sites, and processes to be considered at those sites, as well as various site and process capacity constraints. WRAP sorts out the various allocation options specified by the user and indicates a preferred allocation solution which is the minimum cost plan that meets all the user-supplied constraints. Use of the model enables users to study and analyze the costs and implications of all available alternatives under consideration. WRAP has been used for decisions regarding solid waste management in Massachusetts, in Illinois, and in St. Louis, Missouri.

2. Functional Capabilities: WRAP is an optimizing model which selects, sizes, and locates solid waste processing and disposal facilities. Costs for the solid waste systems are determined by a specialized fixed charge linear programming algorithm. There are two operational modes available: static and dynamic. The dynamic operating mode allows for two to four planning periods. Planning periods are expressed in years, and, in the dynamic mode, are consecutive over the total planning period.

The model consists of a series of equations which consider the sources of solid waste generation, a set of sites, and processes to be considered at those sites, as well as various site and process capacity constraints. The processes can be transfer stations, resource recovery processes (including the extraction of recoverable resources to be marketed), secondary processes (which receive the residue of primary processes as input) and various disposal processes. WRAP further considers many transportation route alternatives from sources of waste generation to sites, and from sites to sites, with due allowance for site traffic constraints.

3. Basic Assumptions: WRAP is a fixed-charge linear programming model, using as the optimizer an algorithm developed by Dr. Warren Walker of Cornell University in Ithaca, New York. The fixed-charge capability of the model permits the representation of economies of scale in process costs. Since the model is cost-minimizing, it will seek out the lowest cost segment at any level of tonnage. Thus the capability of treating cost in two parameters (fixed and variable, or intercept and slope) permits the model to represent economies of scale at any level of accuracy desired. In the actual model applications, three segment representations have been used for nearly all processes.

4. Input and Output: Program execution data is input from a sequential data set, normally the card reader. There are eight types of inputs to be prepared. Five of the input types are required by every program. Three input types are optional. All data for a particular input type is input sequentially. There is no special ordering required within an input type. However, a special ordering is required for the types of user-supplied inputs. The required input sequence follows:

1) Control Records: four control record inputs are possible. Two records are always required and two records are optional.
2) Source Identification Records: an identification record for each original solid waste source must be supplied. Each record must have a unique source identification code as well as the record code.
3) Site Identification Records: there must be one record

for each intermediate and ultimate site. All site records are input in one group.

4) Process Identification Records: there are five types of records possible for each unique process. Though the processes need not be in a particular order, the records associated with each process must be in a specific sequence.

5) Site Process Identification Records: there is one record for each process at each site, and there may be a maximum of 125 records. These records do not need to be in any particular order.

6) Transportation Activity Records: these records are optional, but generally part of the input file. Each record must have an activity type code which describes the transportation links.

7) Truck Constraint Identification Records: these records are optional and are required only when the user's control data indicates that sites are to be subject to truck contraints. There must be one record for each truck constraint, and each record may have a maximum of three site identification codes.

8) Starting Basis Records: these records are optional and are not considered part of the problem identification records. These records are input only when the user has indicated their availability. The number of records is determined by the number of rows (equations) in the matrix.

There are six types of output generated in the WRAP program: (1) optional debugging variables and tables, (2) error messages and codes, (3) input data reports, (4) punched transportation and matrix decks, (5) intermediate phase solution tables, and (6) final solution punchout and reports.

5. System Resource Requirements: The WRAP program does not require any specialized computer environment. The program, however, is very large and does require special handling at execution time. Memory requirements for the 90 (equations) x 360 (coefficients) matrix WRAP model are 270K bytes of storage. This requirement must be modified if the model dimensions are altered to accomodate a larger matrix which uses more memory or to process a smaller matrix which uses less computer memory. The input-output file requirements are: a card reader, a card punch, at least one printer, and a disk with storage for at least eight files. An environmental engineer or programmer familiar with computer modeling is needed to fulfill the manpower requirements for the WRAP program.

6. Applications: WRAP has been used in several locations by decision-makers who are considering regional solid waste management. In Massachusetts, the model was used to identify the most efficient regional system design for that state's first regional resource recovery system. WRAP was used in St. Louis, Missouri, to determine the advantages of community participation in a proposed regional solid waste management plan. In suburban Chicago, WRAP was used to evaluate the economic feasibility of various solid waste management and recovery options facing the decision-makers.

7. Technical Contact

Frank McAlister (WH-563)
U.S. Environmental Protection Agency
Office of Solid Waste
401 M Street, S.W.
Washington, D.C. 20460

FTS: 382-2223 COM: 202/382-2223

8. References

Berman, Edward B., et al. "WRAP: A Model for Regional Solid Waste Management Planning - User's Guide." Publication No. EPA/530/SW-574, prepared by the Mitre Corporation, Bedford, Massachusetts, under Contract No. 68-01-2976, February 1977.

Hensey, Verniece, et al. "WRAP: A Model for Regional Solid Waste Management Planning - Programmer's Manual." Publication No. EPA/530/SW-573, prepared by the Mitre Corporation, Bedford, Massachusetts, under Contract No. 68-01-2976, February 1977.

ATMOSPHERIC DISPERSION OF RADIONUCLIDES (AIRDOS-EPA)

1. Model Overview: AIRDOS-EPA is a model for estimating annual intakes and exposures from the atmospheric release of radionuclides. The purpose of the program is to provide these quantities as input to a companion program (DARTAB) to assess the individual or collective doses and risks associated with chronic releases of radionuclides. The model is a revision of AIRDOS-II (Mo77). Atmospheric dispersion, wet and dry deposition, and food pathway models are included. Provision is made for radionuclide chain ingrowth and decay as well as environmental removal in the terrestrial portion of the model.

2. Functional Capabilities: AIRDOS-EPA calculates radionuclide concentrations in air and on the ground surface and intake rates for inhalation and ingestion. Calculations can be performed for an individual at the grid locations or for a population distributed over the grid. Releases of up to 36 radionuclides from as many as 6 (point or area) sources can be considered. All sources are located at the origin of the calculational grid. Up to 320 or 400 locations may be described by the circular and square grid options respectively. All quantities calculated are long-term averages. Source terms are specified in curies/year. Air and ground surface concentrations are in curies/cubic meter and curies/square meter respectively. Ingestion and inhalation intake rates are in pico curies/year. The concentration of the short-lived progeny of radon-222 is in working levels. Concentration and intake rate calculations are performed after a user specified period of operation at the specified release rates.

3. Basic Assumptions: Dispersion is calculated by a straight line, long-term average, Gaussian model. Momentum or buoyant plane rise can be calculated or assigned a value for each stability class. A dry deposition velocity and a precipitation scavenging rate can be specified for each radionuclide. A source depletion model accounts for plume depletion due to deposition. The terrestrial model includes environmental removal as well as a radiological decay. The food pathway model (vegetable, meat, and milk) is consistent with that in Reg. Guide 1.109 (NRC77). Ingrowth for radionuclide chains subsequent to deposition can be calculated by providing a set of ingrowth factors. Air concentrations of short-lived radon-222 progeny are calculated in working level units for a specified value of equilibrium. Output for DARTAB is in an unformatted file. The basic calculational methodology is from AIRDOS-II (Mo77) with modifications for area sources, radon progeny concentrations, terrestrial ingrowth for radionuclide chains and an updated food pathway model.

4. Input and Output: Model inputs include: grid size values; wind data; stack or area source data; radionuclide release rates, deposition and settling velocities, scavenging rates, and decay constants; arrays of meat animals, dairy cattle, crop areas, and population data for each grid location; the fraction of each food category consumed from outside the assessment area; the fraction of that consumed food which is produced within the assessment area which is in the grid location; ingestion; agricultural model parameters; ingestion rates by food category; inhalation rate; radionuclide decay and environmental removal rate constants of soil to vegetation; intake to meat and intake to milk conversion factors; radionuclide chain ingrowth factors; clearance class; and gastro intestinal absorption fraction.

Printed outputs available include: predicted air concentrations; dry and wet deposition rates for each location and radionuclide; ground-level Chi/Q for each location by radionuclide; agricultural and population data for each grid location; list of nuclide independent variables; list of computer totals of population, food production, and food consumption for the assessment area; a list of nuclide dependent data for each nuclide; individual or population weighted concentration and intake rates for each location by nuclide, radon-222 progency concentration for each location; and dose summaries (supplementary - not used for AIRDOS-EPA/DARTAB assessments). An unformatted file is created of concentration and intake for each location to be used with DARTAB for a dose and risk assessment.

5. Computational System Requirements:

This system may be run on an IBM 360 or 370 series or an equivalent. It is coded in FORTRAN IV (H extended)

6. Applications: This model provides a means for the radiological assessment of radionuclides released to the atmosphere. It has been used by EPA and the Oak Ridge National Laboratory for this purpose. The model is generally used in conjunction with DARTAB for dose and risk assessments.

7. Contact:

David Fields
Oak Ridge National Laboratory
P.O. Box X
Oak Ridge, TN 37830
COM: (615) 576-2131

8. References:

Begovich, C.L., E.C. Schlatter, S.Y. Ohr, K.R. Eckerman, "DARTAB: A Program to Combine Airborne Radionuclide Environmental Exposure Data with Dosimetric and Health Effects Data to Generate Tabulations of Predicted Impacts." ORNL-5692, 1980.

Mo77 Moore, R.E. "The AIRDOS-II Computer Code for Estimating Radiation Dose to Man from Radionuclides in Areas Surrounding Nuclear Facilities." ORNL-5245, 1977.

Mo79 Moore, R.E. "AIRDOS-EPA: A Computerized Methodology for Estimating Environmental Concentrations and Dose to Man from Airborne Releases of Radionuclides." EPA 520/1-79-009, ORNL-5532, 1979.

NRC77 U.S. Nuclear Regulatory Commission, Regulatory Guide 1.109, Calculation of Annual Doses to Man from Routine Releases of Reactor Effluents for the Purpose of Evaluating Compliance with 10 CFR Part 50, Appendix I. (Revision 1). Office of Standards Development, 1977.

GREAT LAKES DOSE/CONCENTRATION (GLA-1)

1. Model Overview: This model uses a simplified representation of the Great Lakes along with the time dependent dose equations of International Commission on Radiological Protection (ICRP) 10A to predict ambient lake concentrations on the dose rates resulting from chronic ingestion of radioactivity in lake waters. The program is also applicable to other pollutants.

2. Functional Capabilities: The model comprises a simplified physical representation of the Great Lakes chain which considers only total volume of each lake, assumes annual mixing but allows for changes in dilution volume required by thermoclines, and corrects for sedimentation and equilibration where required. Dose rates due to chronic ingestion of 2.2 liters of water per day are calculated according to ICRP 10 and ICRP 10A.

3. Basic Assumptions: GLA-1 assumes constant total volume, constant outflow and inflow, and constant surface area. It assumes that thermocline exists for 1/2 year at a depth of 17 meters and that inflow and outflow are from the epilimnion during this period but that perfect mixing occurs during the balance of the year. Concentration equations are convoluted with the ICRP equation for organ burden and solved in closed form. Only six isotopes, Tritium (H-3), Cobalt-60 (Co-60), Strontium-90 (Sr-90), Cesium-134 (Cs-134, and Cesium-137 (Cs-137) are treated at present.

4. Input and Output: Major inputs to te GLA-1 include source terms, time results desired, initial conentrations, and lake volumes and outflows. As currently progammed, individual sources discharging into lakes can be usd or parameters for

sets of nuclear power plants having differing types of rad waste systems may be substituted.

Outputs are lake concentrations for the five isotopes at each time specified along with dose rate and dose equivalents. Concentrations as a function of time for other pollutants can be found without altering the program. Degradable pollutants can be treated like radionuclides by selection of an appropriate decay constant.

5. System Resource Requirements: All programs are written in FORTRAN for an IBM 360/370 system. The model requires 150K bytes of core memory. A background in computer programming is useful in using this model.

6. Applications: GLA-1 has been used to predict concentrations and doses from Great Lakes waters due to nuclear fuel cycle activities projected through the year 2050.

7. Technical Contact

R. E. Sullivan
U.S. Environmental Protection Agency
Criteria and Standards Division
Crystal Mall #2
1921 Jefferson Davis Highway
Arlington, VA 22202
COM 703/557-9380 FTS 557-9380

8. References

Sullivan, R.E. and Ellett, W.H. The Effect of Nuclear Power Generation on Water Quality in the Great Lakes. ORP/CSD-77-5, 1977.

HIGH LEVEL RADIOACTIVE WASTE REPOSITORY RISK MODEL (REPRISK)

1. Model Overview: This computer code calculates the expected genetic and somatic health effects at a generic high level radioactive waste geologic repository. The code calculates radionuclide releases to air, land surface, and rivers or lakes from a repository as a result of expected events and accident events. The accidents are human intrusion (drilling), breccia pipes, faults, meteorites and volcanoes. The expected events are shaft and borehole leakage and bulk rock transport. The releases result either from destruction of waste packages or disturbance of the contaminated repository backfilled tunnels. The concentration of radioactivity in the backfilled tunnels depends on availability of water in the tunnels, the dissolution of radionuclides (solubility), and the characteristics of the waste matrix and canisters. Movement of contaminated water in the tunnels is either directly to land surface or to aquifers overlying the repository. Movement of the radioactivity in the aquifer is governed by groundwater flow and retardation of radionuclides.

2. Functional Capabilities: The model calculates the total release of radionuclides over a time period and converts these releases to health effects. To calculate releases the flow rate of radioactivity in curies per year is integrated either analytically or numerically over the time period of interest. The numerical integrator is 90% accurate. Flow in the aquifer is 1-dimensional nondispersive. The tunnel mixing volume is assumed homogeneous. Parameters are constant over all time, but flow rates of water from the repository are time dependent. The health effects are combined with event probabilities to calculate probability consequence curves and overall risk.

3. Basic Assumptions:

1) One-dimensional non-dispersive aquifer

2) Homogeneous mixing volumes whose radionuclide concentrations can be described by first order differential equations.

3) Input parameters are constant over all time.

4) Probabilities of accident events are constant over various time bands. A reasonable number of time bands can be input.

4. Input and Output: Representative input data will be contained in the two EPA documents listed in the references section.

Two types of output are available for somatic health effects, genetic health effects, or release limit ratios: 1) Integrated risk or release limit ratios and 2) Probability consequence curves.

5. System Resource Requirements: REPRISK can be run on an IBM 370. The model is currently stored on two magnetic tapes and requires a line printer for output.

6. Applications: EPA/ORP is using the code to conservatively evaluate 5 generic high level waste repositories - bedded salt, granite, shale, and basalt. This effort supports the EPA/ORP EIS and standard for high level waste repositories.

7. Technical Contact

Daniel J. Egan
U.S. Environmental Protection Agency
Criteria and Standards Division
Crystal Mall #2
1921 Jefferson Davis Highway
Arlington, Va. 22202
COM 703/557-8610 FTS 557-8610

8. References

User's Manual to be published.

Smith, C. B.; Egan, D. J.; Williams, W. A.; Gruhlke, J. M.; Hung, C-Y; and Serini, B. Population Risk from Disposal of High-Level Radioactive Wastes in Geologic Repositories. EPA/520/3-80-006.

Smith, J.M., Fowler, T.W., and Goldin, A.S. Environmental Pathway Models for Evaluating Population Risks from Disposal of High-Level Radioactive Wastes in Geologic Repositories. EPA 520/5-80-002.

MAXIMUM INDIVIDUAL DOSE MODEL (MAXDOSE)

1. Model Overview: The Maxdose code is a Gaussian dispersion model that calculates accidental releases from a nuclear waste repository. Both geological and human events are modelled. Each event produces a given set of dose rates at different times and distances. A second set of tables estimates contaminated areas and individual risk. Both leaching and dissolution remove wastes from the matrix into the accessible environment. The releases are used to calculate the dose table.

2. Functional Capabilities: The code can calculate the dose for up to 10 distances, 13 dose times, and 20 nuclides per run. All transport models are 2-dimensional, yielding the highest dose along the centerline. Error on numerical integration is less than 10% using cautious adaptive Romberg extrapolation.

3. Basic Assumptions: For atmospheric release, MAXDOSE uses AIRDOSE equations and no direction is specified for the wind. Water releases are calculated along the centerline, where the maximum concentration occurs. Area calculations assume parabolic distribution for contaminants in the groundwater and a circular distribution for air release.

4. Input and Output: Input to the model includes initial inventories of waste, their halflives, retardation factors, 3 sets of dose conversion factors, solubilities, bioaccumulation factors, permeability and its rate of change, numerical constants for approximating the gradient, the canister life, leach rate, groundwater velocity, size of tank, porosities,

dose times, and distances. The boreholes and the flow through the boreholes are modeled.

Output consists of an echo check of the input data in a standard format. A table of dose rates at various dose times and distances, and areas contaminated by a given event are presented.

5. System Resource Requirements: MAXDOSE is coded in FORTRAN and is run on an IBM 360 mainframe. A subroutine of this model calls a routine, TIMER, that is coded in machine language. Engineering and programming backgrounds, and knowledge of the job control language of the International Mathematics and Statistics Library (IMSL) are useful.

6. Applications: Two routines, CTIME and DCADRE, are not in the code. They are in the linkage step of the job control language. DCADRE is a numerical integration from the International Mathematics and Statistics Library. CTIME returns the time of day and date the job is run. The code has been used to estimate risks to individual and in IDAR (Individual Dose Assessment Report).

7. Technical Contact

Barry L. Serini
U.S. Environmental Protection Agency
Office of Air Noise and Radiation
Criteria Standards Division
Crystal Mall #2
1921 Jefferson Davis Highway
Arlington, VA 22202

8. References

MAXDOSE - EPA User's Manual

NONIONIZING RADIATION MODELS

1. Model Overview: Certain mathematical models have been developed to assist researchers involved in the biological effects of nonionizing electromagnetic energy in the RF-microwave frequency spectrum. Such models have provided some insight into the intersection of RF energy with biological objects (e.g., experimental animals, human subjects, etc.) and have provided significant data on average and localized energy absorption rates in such objects. These data enable researchers to predict approximately the thermal load to which an animal is being subjected during experimental irradiation and to extrapolate research findings to humans. This summary primarily discusses modeling work performed in-house within EPA or under EPA grants; similar work sponsored by other government agencies has been recently summarized in the form of a dosimetry handbook. XSECT and ECOMP programs were developed at the RAND Corporation, Santa Monica, Calif.; EPA obtained copies of these in 1972. The variations on ECOMP were developed in-house at Research Triangle Park, N.C. EBCO was developed under EPA grant at Oregon State University.

2. Functional Capabilities: The EPA models examine the interaction between a plane electromagnetic wave and biological objects composed of dissipative (lossy) dielectric materials which possess a simple spherical or prolate spheriodal shape. The model employing a spherical object will be discussed first.

The spherical model actually consists of a core of brain-like material surround by thin concentric layers of other tissues including cerebro-spinal fluid, dura, bone, fat and skin. The model is a crude approximation to isolated animal and human heads. Because of the chosen spherical boundaries of the dielectric object, the mathematical solution to the electro-magnetic problem is readily formulated using the Mie theory. The basic solution involves expanding the incident and secondary (scattered and internally induced) fields into vector spherical harmonics involving spherical Bessel functions of complex argument. The problem has been programmed in FORTRAN for computational solution . on both IBM 360/50 and UNIVAC 1110 machines. Two basic programs have been written for this problem: XSECT computes the absorption efficiency (electromagnetic absorption cross section divided by geometric cross section) of a given sized sphere over a given range of incident frequencies, as well as the overall specific absorption rate (SAR) or dose rate, averaged throughout the model. The other program, ECOMP, computes the local internal electric field strength as well as the local SAR value at various defined locations within the sphere, for a given incident frequency. Two additional programs both employing ECOMP have been developed: PLOT is a graphical routine giving plots of local SAR against radial distance for different azimuthal angles. ECOMX searches for the peak internal SAR value over a given range of RF frequencies for a given sized sphere. Convergence tests are employed in these programs in order to ensure that there is rapid convergence of the infinite series used in the Bessel function expressions. Convergence is generally obtained within 12-15 terms. Valid solutions are obtainable for all combinations of sphere size and wave length including the important resonant region where energy absorption reaches a peak.

The prolate spheriodal model is composed of homogeneous muscle-like dielectric only and simlulates large-scale objects such as humans or primates. Solutions to the problem are based on the extended boundary condition method (EBCM) which has been found to be the most successful of the various methods available for dealing with lossy prolate spheroid objects. However, for spheroids having high eccentricity ratios equivalent to that of standard man (a/b = 6.3), the mothod breaks down in the resonant frequency region owing to problems of ill-conditioned matrices which the computer cannot handle. The computer program, EBCO, is written in FORTRAN and has been run on a Control Data CYBER 70, Model 73 machine.

3. Basic Assumptions: The electromagnetic radiation is assumed to be a simple plan wave, as exists in the far-field of an antenna. The biological objects are of simple spherical or prolate spheroid shape and are composed of dissipative dielectric materials that are linear, homogeneous and isotropic. The heat transfer or conduction aspects of the problem have not been considered.

4. Input and Output:

a. Inputs for sphere model.
   1) Radius of core.
   2) Number of outer layers and layer thicknesses.
   3) Dielectric data (relative permittivity and conductivity) of all tissue equivalent materials as a function of frequency.
   4) Frequency or frequency range of incident wave.
   5) Internal spherical co-ordinates, (r , θ , ϕ) at which internal fields are to be computed (or range of same).
   6) Maximum allowable number of terms in series and tolerance for convergence of series.

b. Inputs for prolate spheroid model.
   1) Major and minor axis values.
   2) Dielectric data of muscle-equivalent material as a function of frequency.
   3) Frequency range of incident wave.
   4) Orientation of major axis of spheriod with respect to E-field vector.
   5) Angle of incident wave with respect to major axis.

c. Outputs for both models.
   1) Absorption cross section and absorption efficiency
   2) Total absorbed power.
   3) Average SAR.

d. Outputs for sphere model only.
   1) Local internal E-field values (r, θ, ϕ components).
   2) Local SAR or dose rate value.

5. System Resource Requirements: All programs are coded in FORTRAN IV or V and require a high-speed computer with approximately 75-80 thousand word capacity. Heavy use is made of double precision arithmetic. Data preparation requires one to two hours, while output analysis may require a day or two, depending on the form of data presentation desired. A person with some background in electro-magnetic theory and scientific programming is helpful.

6. Applications: These models provide insight into the effect of nonionizing electro-magnetic energy in the RF-microwave frequency, and allow researchers to predict approximately the thermal load to which an animal is being subjected to during experimental irradiation. These results can be extrapolated and applied to humans.

7. Technical Contact

Dr. Claude M. Weil
Experimental Biology Division (MD-74)
Health Effects Research Laboratory
Environmental Protection Agency
Research Triangle Park
N.C. 27711
FTS 629-7740 COM 919/541-7740

8. References

Durney, C.H. et. al.,"Radio Frequency Radiation Dosimetry Handbook, Second Edition "Report SAM-TR-78-22, published by USAF School of Aerospace Medicine, Brooks Air Force Base, Texas 78235, May 1978.

Weil, C.M., "Absorption Characteristics of Multilayered Sphere Models Exposed to UHF/Microwave Radiation", IEEE Trans. on Biomed. Eng., BME-22, pp. 468-476, November 1975.

Tripathi, V.K. and Lee, H., Electromagnetic Power Absorption by Prolate Spheroid Models of Man and Animals at and near Resonance, Final Report under EPA Grant No. R-804697-01-1, December 1978.

PLUTONIUM AIR INHALATION DOSE (PAID)

1. Model Overview: The model is designed to calculate dose rates and doses resulting from the acute or chronic lifetime inhalation or ingestion of transuranic radioisotopes.

2. Functional Capabilities: The model is designed for long-lived parents or daughters. Only one daughter is permitted. Gastro-intestinal tract (GIT) and blood transfer fractions are used, but no time delay for either is included.

3. Basic Assumptions: The model is, basically, a combination of the International Commission on Radiological Protection (ICRP) lung model and a standard organ model using exponential retention functions. The resulting solutions are analytical, require no numerical integration, and are obtained rapidly and exactly for the times desired.

4. Input and Output: Input is the acute or chronic intake, deposition fractions for the lung compartments, the mass for post blood organs and physical and biological halflives, transfer fractions, and average energies for the parent and daughter isotopes.

Output is for all input times, the dose rates and doses for each lung compartment, including lymph nodes, and for the reference organs. The values for the trachiobronchial compartment due to clearance from the pulmonary are also given explicitly.

5. System Resource Requirements: PAID is coded in FORTRAN and is run on an IBM 360/370 system. Any standard model printer can be used. Operation requires a computer programmer.

6. Applications: The model has been used to calculate lung and organ doses for transuranic and other radioisotopes. It is used primarily by ORP/EPA.

7. Technical Contact

R. E. Sullivan
U.S. Environmental Protection Agency
Criteria and Standards Division
Crystal Mall #2
1921 Jefferson Davis Highway
Arlington, VA 22202
703/557-9380

8. References

Sullivan, R.E. PAID: A Code for Calculating Organ Doses Due to the Inhalation and Ingestion of Radioactive Aerosols. ORP/CSD-77-4, 1977.

RADIONUCLIDE DOSE RATE/RISK (RADRISK)

1. Model Overview: RADRISK is a model designed to estimate the health risk due to inhalation or ingestion of radionuclides for arbitrary exposure periods. The end result of the system is a set of values relating fatal cancers and genetically significant radiation doses to a unit intake of radionuclides. The model is a greatly revised combination of two previously existing programs, INREM II and CAIRD. The health risk from external exposures is also estimated by the CAIRD model using dose rates from a separate model, DOSFACTER.

2. Functional Capabilities: RADRISK calculates the radiation dose rates and estimated fatal cancers resulting from the chronic inhalation or ingestion of one pico curie/yr of radioisotope. All radioactive decay products of the parent isotope are also considered. Dose rates are calculated over a 110-year period for eighteen organs. Cross irradiation dose rates are incorporated using Monte Carlo results from the S-factor model. These dose rates are then combined in a life table, using U.S. population mortality rates, to compensate for competing risks in estimating radiation health effects. External dose rates, taken from DOSFACTER, are treated similarly in the life table analysis. An integration of the gonadal dose rate is also performed to obtain the 30-year genetically significant dose. Input units are pico curies/yr, pico curies, or squared centimeter pico curies/cubed centimeter. Dose rates are given in mrad/yr for both high-LET and low-LET radiation and the life table returns estimated premature deaths to a cohort of 100,000 for each cancer.

3. Basic Assumptions: The dose rate calculational model incorporates the International Commission on Radiological

Protection (ICRP) lung and gastro-intestinal tract models; and uses exponential retention functions and standard metabolic parameters for the post blood organs. Nonexponential retention functions are fitted, by means of an auxiliary program, to an exponential series of up to five terms. The life table calculation is based on a cohort of 100,000 persons whose mortality rate is that of the U.S. 1969-1971 population. The additional risk, either absolute or relative, from radiation is then followed from birth (0 years) to death (110 years) of the cohort. At present, no age dependence is allowed in the dose rate calculation (a reference man is assumed) although the life table dose rate or risk may be age adjusted.

4. Input and Output: Inputs required for the dose rate portion of the code include the physical (half life, energy) and metabolic (transfer fractions, retention functions) data for the parent and each daughter product. In addition, a library of cross-irradiation terms must be supplied. The life table calculation, in addition to the time dependent dose, requires specification of the risk, including latency and plateau periods, associated with the radiation. For relative risk cases, mortality rates must be supplied for each cancer to be considered.

Outputs comprise the total dose rate, for both high-LET and low-LET radiation, to each of 18 organs at the midpoint of specified time intervals. Options are available for printing out each daughter contribution as well as the cross-irradiation terms. The integrated genetically significant dose to the gonads, along with an average value, is also output. The life table calculation outputs the number of premature deaths, the average years of life lost for each, and the decrease in overall life expectancy for each cancer type as well as the totals.

5. System Resource Requirements: All programs are written in FORTRAN for an IBM 360/370 system. The model requires 500K bytes of core memory. Any standard 132 column printer can be used. Operation requires a background in programming, engineering, and health/medical physics.

6. Applications: This model has been used to produce a set of dose/risk values for a unit intake, or unit exposure, of most common radioisotopes. It has been run extensively at Oak Ridge National Laboratory. The major external link is S-Factor output.

7. Technical Contact

R. E. Sullivan
U.S. Environmental Protection Agency
Criteria and Standards Division
Crystal Mall #2
1921 Jefferson Davis Highway
Arlington, VA 22202
COM 703/557-9380 FTS 557-9380

8. References

RADRISK (to be published)

Dunning, D.E., Jr., *et al*. *S-FACTOR: A Computer Code for Calculating Dose Equivalent to a Target Organ per Microcurie-Day Residence of a Radionuclide in a Source Organ*, 1977.

Cook, J.R., *et al*. *CAIRD: A Computer Code for Cohort Analysis of Increased Risks of Death.* EPA 520/5-78-012, 1978.

Kocher, D.C. DOSFACTER: Dose-Rate Conversion Factors for External Exposure to Photon and Electron Radiation from Radionuclides Occurring in Routine Releases from Nuclear Fuel Facilities. ORNL/NUREG/TM-283, 1979.

Killough, G.G., et al. INREM-II: A Computer Implementation of Recent Models for Estimating the Dose Equivalent to Organs of Man from an Inhaled or Ingested Radionuclide. ORNL/NUREG/TM-84, 1978.

A COMPUTER PROGRAM FOR THE RISK ASSESSMENT OF TOXIC SUBSTANCES (MULTI80G)

1. Model Overview: This program was developed for generating low-dose carcinogenic risk assessments of toxic substances based on the generalized multi-hit and one-hit dose-response functions applied to animal response data derived from lifetime feeding studies.

2. Functional Capabilities: The limitations of the model are:

   1) There must be at least two positive (non-zero) dose level.

   2) There may be no more than 14 positive dose levels.

   3) The average run time may vary for the same job by as much as ±20%.

3. Basic Assumptions: This model is based on a gamma distribution. Individuals interested in the underlying assumptions are referred to the technical contact for copies of theoretical papers underlying the development of this model.

4. Input and Output: The inputs to the model are:

   1) The number of positive (non-zero) dose levels in the bioassay

   2) Magnitude of each dose level

3) Total numbers of animals on test at each dose level

4) Total numbers of animals with tumor types of interest at each dose level

The principal outputs of interest from the model are:

1) A chi-square goodness of fit test

2) An estimate of the number of "hits" required to initiate a carcinogenic response

3) Point estimates and 90, 95, 97.5, 99, and 99.5 lower confidence limits on "virtually safe dose" for risks for 1 in 10 to 1 in 100,000,000

5. System Resource Requirements: This model is coded in FORTRAN G and is run on an IBM 370/168 mainframe. It requires less than 300k bytes of core memory for execution. It uses any 132 position line printer for output.

6. Applications: The model, in conjucntion with a variety of other models, is used to estimate lifetime carcinogenic risks associated with various levels of suspected human carcinogens. The estimates are then included in risk assessments supporting regulatory actions under Section 5 and 6 of the Toxic Substances Control Act.

7. Technical Contact

Gary Grindstaff
U.S. Environmental Protection Agency
Health and Environmental Review Division
401 M Street, S.W.
Washington, D.C. 20460
COM 202/382-3459 FTS 382-3459

8. References

Rai, K. and Van Ryzin, J. MULTI80: A Computer Program for Risk Assessment of Toxic Substances. Technical Report No. N-1512-NIEHS, Rand Corporation, Santa Monica, 1980.

Van Ryzin, J. and Rai, K. The Use of Quantal Response Data to Make Predictions. In *The Scientific Basis of Toxicity Assessment*. H. Witschi (ed.) Elsevier/North Holland, New York, 273-290, 1980.

Rai, K. and Van Ryzin, J. A Generalized Multihit Dose Response Model for Low-dose Extrapolation. *Biometrics* *36* (to appear), 1980).

A user's manual is available from the technical contact.

ENVIRONMENTAL PARTITIONING MODEL (ENPART)

1. Model Overview: This generalized partitioning model integrates information about a chemical's production, use, and disposal with laboratory data describing its physiochemical properties in order to provide insight into the dominant processes responsible for that substance's transport and degradation in the environment. It is intended to be used in early stages of chemical risk assessments to identify environmental media through which exposure may occur, and to provide a guide for further assessment by indicating the media with the highest exposure potential. The methodology explicitly treats transfer between and transformation within environmental media, and it ranks media as to their exposure potential and transformation processes as to the relative importance in controlling the level of exposure. The analysis can also be applied in the design of a cost-effective testing approach to yield data on interrelated transport and transformation processes which, when considered together, present a clear picture of a substance's environmental fate.

2. Functional Capabilities: The equilibrium partitioning segment of the model combines information on chemical releases and intermedia transport processes to determine the partitioning of the chemical between air, water, soil, sediment, and biota. The dynamic partitioning segment sums the first-order degradation rates to yield the overall transformation half-life for each medium. This is then compared with the previously calculated intermedia transfer half-life to determine if the chemical is degraded before it can be transferred from the media to which it is released.

3. Basic Assumptions: The approach used in the equilibrium partitioning analysis assumes that each medium compartment is homogeneously well mixed, and that all compartments are in equilibrium. The dynamic partitioning portion of the model assumes that inter-compartmental transfer is at a steady state with the transformation processes such as photolysis, hydrolysis, oxidation, and biodegradation. The concentration ratios are determined using fugacity constants describing tendencies to transfer between compartments which are valid for use at low environmental concentrations.

4. Input and Output: The equilibrium partitioning of the model requires data on the substance's vapor pressure, water solubility, soil and/or sediment adsorption coefficients, and the octanol/water partition coefficient, or data for chemical surrogates. The dynamic partitioning portion requires first order or pseudo first order rate constants for major chemical transformation processes. These include ozone and hydroxyl radical oxidation, direct photolysis, aqueous photolysis, hydrolysis in surface water and soil water, and biodegradation in water and soil. The Office of Toxic Substances is in the process of compiling some of this data for major organic chemicals to interface with the computerized version of the model

The model provides the ratios of chemical concentrations between media compartments, rather than absolute concentrations. This avoids the problem of selecting media volumes for the compartments, but allows medias to be ranked in order of exposure potential. Overall environmental persistence of the substances is calculated based upon the degradation and intermedia transfer rates.

5. System Resource Requirements: ENPART is coded in FORTRAN. It can be run using a calculator or VAX 11/780 mainframe. It would be useful for the operator to have basic scientific skills.

6. Applications: The environmental partitioning model is still under development at this writing by the EPA Office of Toxic Substances, Exposure Evaluation Division. It has not yet been used except in test runs. Reference 1 includes a user workbook which allows users to perform model operations using a hand held calculator. A computerized version will become fully operational in 1981, and will be linked to computerized techniques for estimating some input parameters based on data for the chemical of interest or similar ones.

7. Technical Contact

William P. Wood
U.S. Environmental Protection Agency
Exposure Evaluation Division
401 M Street, S.W.
Washington, D.C. 20460
COM 202/382-3928 FTS 382-3828

8. References

Chemical Fate Branch Modeling Team, "An Environmental Partitioning Model (draft)", EPA Office of Toxic Substances, April 1980.

Mackay, Donald, "Finding Fugacity Feasible", Environmental Science and Technology, Vol. 13, No. 10, October 1979, pp. 1218-1223.

EXPOSURE ANALYSIS MODELING SYSTEM (EXAMS)

1. Model Overview: EXAMS is designed for rapid screening and evaluation of the behavior of synthetic organic chemicals in aquatic ecosystems. Starting from a description of the chemistry of a compound, and the relevant transport and physical/chemical characteristics of the ecosystem, EXAMS computes:

1) Exposure: The ultimate (steady-state) expected environmental concentrations (EECs) resulting from a specified pattern of (long term, time-invariant) chemical loadings.

2) Fate: The distribution of the chemical in the system, and the fraction of the loadings consumed by each transport and transformation process.

3) Persistence: The time required for effective purification of the system (via export/transformation processes) should the chemical loadings terminate.

The EXAMS program is an interactive modeling system that allows a user to specify and store the properties of chemicals and ecosystems, modify the characteristics of either, via simple English-like commands, and conduct efficient, rapid evaluations and error analyses of the probable aquatic fate of synthetic organic chemicals.

EXAMS combines the loadings, transport, and transformations of a chemical into a set of differential equations by using the law of conservation of mass as an accounting principle. This law accounts for all the chemical mass entering and leaving a system as the algebraic sum of (1) external loadings, (2) transport processes that export the compound from the system, and (3) transformation processes within the system that convert the chemical to daughter products. The equations used in the program describe the rate of change in chemical concentrations as a balance between increases, originating from external and internally recycled loadings, and decreases resulting from transport and transformation processes.

EXAMS environmental data are contained in a file composed of concise ("canonical") descriptions of the aquatic systems of interest to a user. Each water-body is represented via a set of N segments or distinct zones in the system. The program is based on a series of mass balances that give rise to a single differential equation for each segment. Working from the transport and transformation process equations, EXAMS compiles an equation for the net rate of change of chemical concentration in each segment. The resulting system of N differential equations describes a mass balance for the entire system. EXAMS has been designed to accept standard water-quality parameters and system characteristics that are commonly measured by limnologists throughtout the world. EXAMS also includes a descriptor language that simplifies the specification of system geometry and connectedness. The EXAMS code has been written in a general (N-compartment) form. The software is available in 10-, 50-, and 100- segment versions.

2. Functional Capabilities: The set of unit process equations used to compute the kinetics of chemicals is the central core of EXAMS. These unit models are all "second-order" or system-independent equations. Each includes a direct statement of the interactions between the chemistry of a compound and the environmental forces that shape its behavior in aquatic systems. Most of the process equations are based on standard

theoretical constructs or accepted empirical relationships. For example, the light intensity in the water column of the system is computed using the Beer-Lambert law, and temperature corrections for rate constants are computed using Arrhenius functions.

Ionization of organic acids and bases, and sorption of the compound with sediments and biota, are treated as thermodynamic properties or (local) equilibria that constrain the operation of the kinetic processes. For example, an organic base in the water column may occur in a number of molecular species (as dissolved ions, sorbed with sediments, etc.), but only the uncharged, dissolved species can be volatilized across the air-water interface. EXAMS allows for the simultaneous treatment of up to 15 molecular species of a compound. These include the parent uncharged molecule, and singly or doubly charged cations and anions, each of which can occur in a dissolved, sediment-sorbed, or biosorbed form. The program computes the fraction of the total concentration of a compound that is present in each of the 15 molecular structures (the "distribution coefficents," ALPHA). These values enter the kinetic equations as multipliers on the rate constants. The program thus completely accounts for differences in reactivity that depend on the molecular form of the chemical. EXAMS makes no intrinsic assumptions about the relative transformation reactivities of the 15 molecular species. These assumptions are under direct user control through the way the user structures the chemical input data.

EXAMS computes the kinetics of transformations due to direct photolysis, hydrolysis, biolysis, and oxidation reactions. The input chemical data for hydrolytic, biolytic, and oxidative reactions can be entered either as single valued, second-order rate constants, or as pairs of values defining the rate constant as a function of the environmental temperature specified for each segment.

EXAMS includes two algorithms for computing the rate of photolytic transformation of a synthetic organic chemical. These algorithms were structured to accommodate the two more common kinds of laboratory data and chemical parameters available to describe photolysis reactions. The simpler of the algorithms (subroutine PHOTO1) requires only an average pseudo-first-order rate constant (KDPG) applicable to near-surface waters under cloudless conditions at a specified reference latitude (RFLATG). In order to give the user control of reactivity assumptions, KDPG is coupled to user-supplied (normally unit-valued) reaction quantum yields (QUANTG) for each molecular species of the compound. The more complex algorithm (subroutine PHOTO2) computes photolysis rates directly from the absorption spectra (molar extinction coefficients, ABSG) of the compound and its ions, measured values of the reaction quantum yields, and the environmental concentrations of competing light absorbers (chlorophyll, suspended sediments, dissolved organic carbon, and water).

The total rate of hydrolytic transformation of a chemical is computed by EXAMS as the sum of three contributing processes. Each of these processes can be entered via simple rate constants, or as Arrhenius functions of temperature. The rate of specific-acid catalyzed reactions is computed from the pH of each sector of the ecosystem, and specific-base catalysis is computed from the environmental pOH data. The rate data for neutral hydrolysis of the compound is entered as a set of pseudo-first-order rate coefficients (or Arrhenius functions) for reaction of the 15 (potential) molecular species with the water molecule.

EXAMS allows the user to compute biotransformation of the chemical in the water column, and in the bottom sediments, of the system as entirely separate functions. Both functions are second-order equations that relate the rate of biotransformation to the size of the bacterial population actively degrading the compound. The second-order rate constants (KBACWG for the water column, KBACSG for benthic sediments) can be entered either as single-valued constants or as functions of temperature. When a non-zero value is entered for the Q-10 of a biotransformation (parameters QTBAWG and QTBASG respectively), KBAC is interpreted as the rate constant at 20 degrees C., and the biolysis rate in each sector of the ecosystem is adjusted for the local temperature (BIOTMG).

Oxidation reactions are computed from the chemical input data and the total environmental concentrations of reactive oxidizing species (alkylperoxy and alkoxyl radicals, etc.) specified by the user. The chemical data can again be entered either as simple second-order rate constants, or as Arrhenius functions.

Internal transport, and export, of a chemical occur in EXAMS via advective and dispersive movement of dissolved, sediment-sorbed, and biosorbed materials, and by volatilization losses at the air-water interface. EXAMS provides a set of vectors (JFRADG, etc.) that allows the user to specify the location and strength of both advective and dispersive transport pathways. Advection of water through the system is then computed from the water balance, using hydrologic data (rainfall, evaporation rates, streamflows, groundwater seepages, etc.) supplied as part of the definition of each environment. Dispersive interchanges within the system, and across system boundaries, are computed from the characteristic length (CHARLG), cross-sectional area (XSTURG), and dispersion coefficient (DSPG) specified for each active exchange pathway. EXAMS can compute transport of a chemical via whole-sediment bedloads, suspended sediment wash-loads, ground-water infiltration, transport through the thermocline of a lake, losses in effluent streams, etc. Volatilization losses are computed using a two-resistance model. This computation treats the total resistance to transport across the air-water interface as the sum of resistances in the liquid and vapor phases immediately adjacent to the interface.

External loadings of a chemical can enter the ecosystem via point sources (STRLDG), non-point sources (NPSLDG), dry fallout or aerial drift (DRFLDG), atmospheric wash-out (PCPLDG), and via ground-water seepage (IFLLDG) entering the system. Any type of chemical load can be entered for any system segement, but the program will not implement a loading that is inconsistent with the system definition. For example, the program will automatically cancel a PCPLD entered for the hypolimnion or benthic sediments of a lake ecosystem. When this type of corrective action is executed, the change is reported to the user via an error message.

3. Basic Assumptions: EXAMS has been designed to evaluate the consequences of long-term, time-averaged toxicant loadings that ultimately result in trace-level contamination of aquatic systems. EXAMS generates a steady-state, average flow field for the ecosystem. The program thus cannot evaluate the transient concentrated EECs that arise, for example, from chemicals spills. This limitation derives from two factors. First, a steady flow field is not always appropriate for evaluating the spread and decay of a major pulse (spill) input. Second, the assumption of trace-level EECs, which can be violated by spills, has been used to design the process equations used in EXAMS. The following assumptions were used to build the model:

(1) A first-order evaluation can be executed independently of the chemical actual effects on the system. In other words, the chemical does not itself radically change the environmental variables that drive its transformations. Thus, for example, an organic acid or base is assumed not to change the pH of the system;

the chemical is assumed to not itself absorb a significant fraction of the light entering the system; bacterial populations do not grow (or decline) simply due to the presence of the chemical.

(2) EXAMS uses linear sorption isotherms, and second-order (rather than Michaelis-Menten-Monod) expressions for biotransformation kinetics. This approach is known to be valid for low concentrations of pollutants; its validity at high concentrations is less certain. EXAMS controls its computational range to ensure that the assumption of trace-level concentrations is not grossly violated. This control is keyed to aqueous-phase (dissolved) residual concentrations of the compound; EXAMS aborts any analysis generating EECs that exceed 50% of the compound's aqueous solubility or 1.E-05 in an unionized molecular species. This restraint incidentally allows the program to ignore precipitation of the compound from solution, and precludes inputs of solid particles of the chemical.

(3) Sorption is treated as a thermodynamic or constitutive property of each segment of in the system, that is, sorption/desorption kinetics are assumed to be rapid compared to other processes. The adequacy of this assumption is partially controlled by properties of the chemical and system being evaluated. Extensively sorbed chemicals tend to be sorbed and desorbed more slowly than weakly sorbed compounds; desorption half-lives may approach 40 days for the most extensively bound compounds. Experience with the program has indicated, however, that strongly sorbed chemicals tend to be captured by benthic sediments,

where their release to the water column is controlled by benthic exchange processes. This phenomenon overwhelms any accentuation of the speed of processes in the water column that may be caused by the assumption of local equilibrium.

4. Input and Output: Input parameters include:

(1) A set of chemical loadings on each sector of the ecosystem.

(2) Molecular weight, solubility, and ionization constants of the compound.

(3) Sediment-sorption and biosorption parameters: Kp, Koc or Kow, biomasses, benthic water contents and bulk densities, suspended sediment concentrations, sediment organic carbon, and ion exchange capacities.

(4) Volatilization parameters: Henry's Law constant or vapor pressure data, windspeeds, and reaeration rates.

(5) Photolysis parameters: reaction quantum yields, absorption spectra, surface scalar irradiance, cloudiness, scattering parameters, suspended sediments, chlorophyll, and dissolved organic carbon.

(6) Hydrolysis: 2nd-order rate constants or Arrhenius functions for the relevant molecular species; pH, pOH, and temperatures.

(7) Oxidation: rate constants, temperature, and oxidant concentrations.

(8) Biotransformation: rate constants, temperature, total and active bacterial population densities.

(9) Parameters defining strength and direction of advective and dispersive transport pathways.

(10) System geometry and hydrology: volumes, areas, depths, rainfall, evaporation rates, entering stream and non-point-source flows and sediment loads, and ground water flows.

Although EXAMS allows for the entry of extensive environmental data, the program can be run with a much reduced data set when the chemistry of a compound of interest precludes some of the transformation processes. For example, pH and pOH data can be omitted in the case of neutral organics that are not subject to acid or alkaline hydrolysis.

The 17 output tables include an echo of the input data, and tabulations giving the exposure, fate, and persistence of the chemical. The program prints a summary report of the results obtained. Printer-plots of longitudinal and vertical concentration profiles can be invoked by the interactive user.

5. System Resource Requirements: EXAMS has been implemented in FORTRAN IV as defined by the ANSI FORTRAN X.39-1966 report. The DEFINE FILE extension of the standard is used for file manipulation, but standard unformatted I/O can be substituted with some sacrifice in speed of execution. An overlay capability is required to implement EXAMS on small computers such as the PDP-11 or HP 3000. EXAMS is available from the EPA Athens Environmental Research Laboratory in either a batch or an interactive version. The batch version requires 64K bytes (overlaid) of memory (for aquatic systems of up to 17

segments); this version does not require mass storage capabilities. The interactive version also requires 64K bytes (overlaid) of memory, plus an additional mass storage capability. The interactive version of EXAMS requires 100K bytes of mass storage for utility files, 2K bytes for each chemical in the active files, and 2.5K bytes for each active defined environment. Execution times range from a few seconds to several minutes depending on the problem to be solved. The software is distributed on magnetic tape; the source code consists of about 16,000 card images.

6. Applications: EXAMS can be used to assess the fate, exposure, and persistence of synthetic organic chemicals in aquatic ecosystems in which the chemical loadings can be time-averaged and residuals are at trace levels. The program has been used, for example, by EPA to evaluate the behavior of relatively field-persistent herbicides. EXAMS has been successfully used to model volatilization of organics in specific field situations, and for a general assessment of the behavior of phthalate esters in aquatic systems. EXAMS has been implemented by a number of manufacturing firms for environmental evaluations of newly synthesized materials and has been used in an academic setting for both teaching and research.

7. Technical Contacts

Lawrence A. Burns
U.S. Environmental Protection Agency
Environmental Systems Branch
Environmental Research Laboratory
College Station Road
Athens, Georgia 30613
FTS 250-3123 COM 404/546-3123

David M. Cline
U.S. Environmental Protection Agency
Automatic Data Processing
Environmental Research Laboratory
College Station Road
Athens, Georgia 30613
FTS 250-3123 COM 404/546-3123

8. References

Baughman, G.L. and Burns, L.A. Transport and Transformation of Chemicals in the Environment: A Perspectve. pp. 1-17. In: O. Hutzinger (ed.) Handbook of Environmental Chemistry., Vol. 2, Part A - Reactions and Processes. Springer-Verlag, 1980.

Burns, L.A., Cline, D.M., and Lassiter, R.R. Exposure Analysis Modeling System (EXAMS): User Manual and System Documentation. (443 pp. In process; supplied with software.), 1982.

Lassiter, R.R., Baughman, G.L. and Burns, L.A. "Fate of Toxic Organic Substances in the Aquatic Environment." pp. 219-246 In: S.E. Jorgensen (ed) State-of-the-Art in Ecological Modeling. Proceedings of the Conference on Ecological Modeling, Copenhagen, Denmark 28 Auguest - 2 September 1978. International Society for Ecological Modelling, Copenhagen, 1978.

Wolfe, N.L. Burns, L.A. and Steen, W.C. Use of Linear Free Energy Relationships and an Evaluative Model to Assess the Fate and Transport of Pnthalate Esters in the Aquatic Environment. Chemosphere 9:393-402, 1980.

A FORTRAN PROGRAM FOR RISK ASSESSMENT USING DOSE-RESPONSE DATA TIME-TO-OCCURRENCE (RANK TIME)

1. Model Overview: The program RANK TIME implements the theory developed in a 1980 paper. by Daffer, Crump, and Masterman entitled, "Asymptotic Theory for Analyzing Dose-Response Surivial Data with Application to the Low-Dose Extrapolation Problem" (to appear in Mathematical Biosciences). It is used for analyzing dose-response time-to-occurence data and for estimating low-dose risks from such data. This method is based on the multi-stage model. The data are derived from lifetime feeding studies with animals, usually rodents.

2. Functional Capabilties: The limitations to the model are:

   1) The number of dose groups must be greater than 2 and less than 10.

   2) The number of animals must not exceed 1000.

   3) The animal death times must not exceed 1000.

   4) The degree of the polynomial must not exceed 11.

   5) The number of animals that die of cancer must be less than 300.

3. Basic Assumptions: This model is a variant of the multi-stage model, with death time included as an additional parameter. The model is mathematically quite complex, so individuals interested in the underlying assumptions are referred to the technical contact for copies of theoretical papers underlying the development of this model.

4. Input and Output: The inputs to the model include:

1) Number of dose groups
2) Number of animals in each treatment group
3) Dosages administered to each treatment group
4) Times of death for which confidence limits are to be computed
5) Time of death of each animal
6) Degree of polynomial of multi-stage model
7) Cutoff time for ignoring cancer deaths
8) Method of ties among cancer deaths

Based on a number of estimates and the asymptotic theory developed in the 1980 Daffer, et al. paper, estimates and confidence limits are calculated for a number of quantities. These include:

1) The risk P(t,d) at time t from dose d
2) The extra risk P(t,d) - P(t,o) at time t from dose d
3) The safe dose corresponding to time t and additional risk
4) The expected fraction of life-shortening by the t from dose d

5. System Resource Requirements: This model is coded in FORTRAN G and is run on an IBM 370/168 mainframe. It requires less than 300k bytes of core memory for execution. It uses any 132 positon line printer for execution.

6. Application: This model is used to estimate lifetime carcinogenic risks associated with various suspected human carcinogens. The model is only used when time-to occurrence data is available from an animal bioassay. The estimates of carcinogenic risk are used in risk assessments supporting regulatory actions under Section 5 and 6 of the Toxic Substances Control Act.

7. Technical Contact

Gary Grindstaff
U.S. Environmental Protection Agency
Office of Pesticides and Toxic Substances
401 M Street, S.W.
Washington D.C. 20460
COM 202/382-3459 FTS 382-3459

8. References

Crump, K.S. Daffer, D.Z. and Masterman, M.D.; (1980) Low-Dose Extrapolation Utilizing Time-to-occurrence Cancer Data. In: Final Report, National Institute of Environmental Health Sciences, Contract No. N01-ES-23133.

Daffer, D.Z., Crump, K.C., and Masterman, M.C. (1980) "Asymptotic Theory for Analyzing Dose-response Survival Data With Application to the Low-dose Extrapolation Problem." Mathematical Biosciences 50, pp. 204-230.

A user's manual is available from the technical contact.

A FORTRAN PROGRAM TO EXTRAPOLATE DICHOTOMOUS ANIMAL CARCINOGENICITY DATA TO LOW DOSES (GLOBAL 79)

1. Model Overview: GLOBAL 79 is a program to analyze dichotomous animal carcinogenicity data. It is assumed that at each dose level, animals have been exposed to a constant dose rate of the agent under test and that some positive responses have occurred. The program calculates maximum likelihood estimates of a multistage dose response function. The user may allow the program to set the degree of the polynomial function to be one less than the number of dose groups, or force the degree of polynomial, or globally maximize the likelihood over polynomials of arbitrary degree. A likelihood ratio test is then performed on the linear polynomial coefficient. Next, lower statistical confidence limits on dose and upper statistical confidence limits on risk are calculated for risk levels of 10 (-1)....10(-8) and other dose levels input by the user. Finally, if requested by the user, the program will conduct a Monte-Carlo goodness of fit test of the model to the experimental data.

2. Functional Capabilities: Limitations of the model are: the number of dose levels must not exceed 19; the number of animals must not exceed 2,000; the number of environmental doses input by the user must not exceed 50; and the number of data sets which may be analyzed in one run must not exceed 1,000.

3. Basic Assumptions: This is a multistage model, the parameters of which are estimated by the method of maximum likelihood. However, the model is mathematically complex, thus rather than list them here, individuals interested in the

assumptions and theory of this model may refer to the technical contact for copies of theoretical papers underlying the development of this model.

4. Input and Output: Inputs to the model include:

1) The number of dose levels

2) Goodness of fit option

3) Number of animals at risk at each dose level

4) Number of animals showing a positive response at each dose level

5) Magnitude of each dose level

6) Model option (multistage, forced stage, global optimization)

7) Degree of polynomial (for forced stage option)

8) Number and level of environmental doses for which risks are to be computed

The principal outputs of the model are:

1) Lower statistical confidence limits for the dose producing extra risks of 10(-1), 10(-2).....10(-8) (virtually safe dose)

2) Upper confidence limits on extra risk for maximum likelihood estimated doses (or other doses which are input by the user) corresponding to increased risks of 10(-1),....10(-8)

5. System Resource Requirements: GLOBAL 79 is coded in FORTRAN G and is run on an IBM 370/168 mainframe. It requires less than 300K bytes of core memory for execution. It uses any 132 position line printer.

6. Applications: This model is used to estimate lifetime carcinogenic risks associated with various suspected human carcinogens. The model is only used with dichotomous data from animal bioassays. The estimates of carcinogenic are used in risk assessments supporting regulatory actions under Sections 5 and 6 of the Toxic Substances Control Act.

7. Technical Contact

Gary Grindstaff
U.S. Environmental Protection Agency
Office of Pesticides and Toxic Substances
401 M Street, S.W.
Washington, D.C. 20460
COM 202/382-3459 FTS 382-3459

8. References

Crump, K.S. "An Improved Procedure for Low-dose Carcinogenic Assessment for Animal Data. Journal of Environmental Pathology and Toxicology (to appear), 1980.

A user's manual is available from the technical contact.

MANTEL-BRYAN LOW-DOSE EXTRAPOLATION MODEL (MANTELAN)

1. Model Overview: This computer model is an implementation of the technique for low-dose extrapolation developed by Mantel, Bohidar, Brown, Ciminera, and Tukey in a 1975 paper entitled "An Improved Mantel-Bryan Procedure for `Safety` Testing of Carcinogens" (This paper is available from the technical contact).

2. Functional Capabilities: The limitations of this model are not well known. The documentation is somewhat sparse.

3. Basic Assumptions: The Mantel-Bryan model is a special case of the well-known probit model. Mantel-Bryan, however, assumes a slope of 1.0. The methods used to estimate the parameters and to place confidence limits on a dose are explained fully in a number of theoretical background papers available from the technical contact.

4. Input and Output: Inputs to the model include:

   1) The assumed slope of the dose-response curve (usually 1.0)

   2) The number of experimental groups (e.g. males, females)

   3) The number of dose levels

   4) The number of confidence limits

   5) The chi-square values for desired confidence limits

   6) The dose levels

7) The titles of experimental groups

8) The number responders, the number at risk for each control and treated group in each experimental group

The principal outputs of this model include lower confidence bounds for the dose at specified attributable risks of 10(-1) to 10(-8). These estimates are presented for all dose groups first and then for successively smaller dose group combinations, eliminating the highest dose on each iteration.

5. System Resource Requirements: MANTELAN is coded in FORTRAN G and is run on an IBM 370/168 mainframe. It requires less than 300k bytes of core memory for execution. It uses any 132 position line printer for output.

6. Applications: This model is used to estimate lifetime carcinogenic risks associated with various suspected human carcinogens. The model is only used with dichotomous data from animal bioassays. The estimates of carcinogenic risk are used in risk assessments supporting regulatory actions under Section 5 and 6 of the Toxic Substances Control Act.

7. Technical Contact

Gary Grindstaff
U.S. Environmental Protection Agency
Health and Environmental Review Division
401 M Street, S.W.
Washington, D.C. 20460
COM 202/755-6841 FTS 755-6841

8. References

Mantel, N., Bohidar, N., Brown C., Ciminera, J., and Tukey, J. "An Improved Mantel-Bryan Procedure for "Safety" Testing of Carcinogens." Cancer Research 34, 865-872, 1975.

A user's manual is available from the technical contact.

ONE-HIT LOW-DOSE EXTRAPOLATION MODEL (ONE HIT MD)

1. Model Overview: This program computes maximum likelihood estimates of the parameters of the one-hit model. Abbott's connection is incorporated so that estimates of increased risk may be generated. The parameters generated by the model are used in the assessment of lifetime carcinogenic risks at low environmental doses.

2. Functional Capabilities: The limitations of the model are:

   1) The numbers of experimental clauses must not exceed 10

   2) The numbers of dose levels must not exceed 20

   3) Other limitations, if any, are unknown

3. Basic Assumptions: According to the theory of the one-hit model, there is some risk of cancer from even a slight exposure to a carcinogen. The probability that a carcinogen at a given dosage will induce cancer in a laboratory animal is stated in the experimental probability law. The detailed, mathematical assumptions underlying this model are provided in the program documentation, available from the technical contact.

4. Input and Output: Inputs to the model include:

   1) Number of experimental groups (e.g., males, females)

   2) Number of dose levels

   3) Chi-square values for derived confidence limits

4) Dose levels

5) Titles of experimental groups

6) Number of responders, number at risk for each control and treated group in each experimental group

The principal outputs of this model include:

1) Lower confidence limits for dose at specified attributable risks of 10(-1) and 10(-8)

2) Lower confidence limits on the one-hit parameter

These estimates are presented for all dose groups first and then for successively smaller dose group combinations, eliminating the highest dose on each iteration.

5. System Resource Requirements: This model is coded in FORTRAN G and is run on an IBM 370/168 mainframe. It requires less than 300k bytes of core memory for execution. It uses any 132 position line printer for output.

6. Applications: This model is used to estimate lifetime carcinogenic risks associated with various suspected human carcinogens. The model is only used with dichotomous data from animal bioassays. The estimates of carcinogenic risk are used in risk assessments supporting regulatory actions under Sections 5 and 6 of the Toxic Substances Control Act.

7. Technical Contacts

Gary Grindstaff
U.S. Environmental Protection Agency
Office of Pesticides and Toxic Substances
401 M Street, S.W.
Washington D.C. 20460
COM 202/382-3459 FTS 382-3459

8. References

General statistics text like:

Neter, J. and Wasserman, W., Applied Linear Statistical Models, Irwin, Inc., 1974.

A user's manual is available from the technical contact.

SEASONAL SOIL MODEL (SESOIL)

1. Model Overview: SESOIL is a statistical mathematical model designed for long-term environmental pollutant fate simulations that can describe: water transport (quality/quantity); pollutant transport/transformation; and soil quantity. Simulations are performed for a user specified soil column (designated as compartment), extending between the ground surface and the lower part of the saturated soil zone of a region. The simulation is based upon a three-cycle rationale, each cycle being associated with a number of processes. The three cycles are the: (1) water cycle which takes account of rainfall, infiltration, exfiltration, surface runoff, evapotranspiration, and groundwater runoff; (2) sediment cycle (not currently operational) which takes account of sediment resuspension (because of wind) and sediment washload (because of rain storms); and (3) pollutant cycle which takes account of convection, volatilization, adsorption/desorption, chemical degradation/decay, biological transformation/uptake, hydrolysis, complexation of metals by organics, and cation exchange.

2. Functional Capabilities: The model calculates seasonal (either annual or monthly) concentrations of pollutants in the soil air, soil water, and sorbed to soil solids in up to three layers of a soil column. The model is potentially useful in studying leaching from waste disposal sites and environmental assessment of chemicals in soil environments.

3. Basic Assumptions: The hydrologic cycle is based on Eagleson's theory, which is a statistical dynamic formulation of vertical water budget at a land-atmosphere interface. The fundamental water balance equation sets infiltration equal to precipitation minus surface runoff which is in turn equal to net evapotranspiration and groundwater recharge and loss.

The pollutant cycle is based on a layer-by-layer mass-balance equation, which is solved for the pollutant concentration in each phase.

4. Input and Output: SESOIL does not require calibration because it uses mainly theoretically derived equations. Input can be input for either annual or monthly simulations. Hydrologic input includes climatic (e.g., average precipitation, depth, average storm duration, number of storms), soil (e.g., density, porosity), and chemical data (e.g., degradation rates, molecular weight, adsorption coefficients).

5. System Resource Requirements: The model has been implemented on a IBM 370 and a VAX 11/780. It is coded in FORTRAN and requires several disk input files.

6. Applications: The SESOIL model predictions have been compared with laboratory determined concentrations in the upper unsaturated zone at two land-treatment sites. Concentrations were found to agree within expected limits.

The model has also been employed as an exposure assessment model for screening, analyzing, and prioritizing pollutant behaviors in a number of soil disposal systems.

The model is still under development and is still being extended under contracts with the Office of Toxic Substances.

7. Technical Contact:

Annett Nold
U.S. Environmental Protection Agency
Office of Toxic Substances
Exposure Evaluation Division (TS-798)
401 M Street, S.W.
Washington, DC 20460
COM 202/382-3926

8. References:

Bonazountas, M. and J. Wagner (1981); "SESOIL: A Seasonal Soil Compartment Model," Arthur D. Little, Inc., Cambridge, Massachusetts 02140. Prepared for U.S. Environmental Protection Agency, Office of Toxic Substances, Contract No. 68-01-6271.

STATISTICAL METHODOLOGY FOR TOXICOLOGICAL RESEARCH (MRST)

1. Model Overview: MRST is a program designed to use both as a powerful research tool and a statistical analyzer of experimental data from toxicological studies. The program will provide a statistical analysis of real experimental data. In addition, the program has the capability of simulating experimental data. This capability is particularly useful in evaluating the effectiveness of the risk estimation procedures and alternative experimental designs, especially with regard to a design's number and spacing of dose levels and the number of test animals assigned to each dose level.

2. Functional Capabilities: The limitations of the model are tied to the input specifications. Given the extent of the required program input, interested users are referred to the technical contact for the program documentation which will cover these specifications in detail.

3. Basic Assumptions: The program is based, to some extent, on the simulation of time-to-death for an experimental animal by a Weibull distribution. However, the theory underlying this model is quite involved. Interested users are referred to the technical contact for copies of the theoretical papers upon which this model is based.

4. Input and Output: The input requirements for this program are quite large, too many to list here in detail. They include detailed information from the bioassay, such as individual animal death times. Interested users are urged to obtain a copy of the input specifications from the technical contact.

The outputs from this model are extremely voluminous and too numerous to list here. In general, estimates of increased risk and life-shortening are provided. Interested individuals are urged to obtain a sample output listing from the technical contact.

5. System Resource Requirements: This model is coded in FORTRAN G and is run on an IBM 370/168 mainframe. It requires less than 300K bytes of core memory for execution. It uses any 132 position line printer for output.

6. Applications: This model is used in conjunction with a variety of other models to estimate lifetime carcinogenic risks associated with various levels of suspected human carcinogens. However, this model is used only with time-to-occurrence dose response data. These estimates are then included in risk assessments supporting regulatory actions under Sections 5 and 6 of the Toxic Substances Control Act.

7. Technical Contact

Gary Grindstaff
U.S. Environmental Protection Agency
Office of Pesticides and Toxic Substances
401 M Street, S.W.
Washington, D.C. 20460
COM 202/382-3459 FTS 382-3459

8. References

Hartley, H.O., and Sielken, R.L. "Estimation of "Safe Dose" in Carcinogenic Experiments".
Biometrics 33 p. 1-30, 1977.

Hartley, H.O. and Sielken, R.L., Jr. "Development of Statistical Methodology for Risk Examination." Final report. National Center for Toxicological Research, Contract No. 222-77-2001 April, 1978.

A users's manual is available from the technical contact.

UNIFIED TRANSPORT MODEL - TOXICS (UTM-TOX)

1. Model Overview: The Unified Transport Model is a multimedia model that simulates the movement of a chemical through an inland watershed. The model calculates the concentration of organic and inorganic chemicals in air, water, soil, sediment and biota. The UTM consists of the Atmospheric Transport Model (ATM), the Wisconsin Hydrologic Transport Model (WHTM), the Terrestrial Ecosystem Hydrology Model (TEHM), and a suite of associated submodels. The model was originally developed by the Oak Ridge National Laboratory to simulate trace element transport through a forested ecosystem. The model was modified by Oak Ridge in 1980-81 for the Environmental Protection Agency to incorporate the transport and transformation processes associated with organic chemicals.

2. Functional Capabilities: The model is applicable to small watersheds consisting of up to 3 land segments and 7 reaches. The concentration of the chemical in air is determined on a monthly basis. Movement of the chemical through the terrestrial and aquatic environment is simulated at 15 minute intervals. The average monthly and annual concentrations can be calculated with an accuracy of better than an order of magnitude. The hydrologic submodel requires calibration.

3. Basic Assumptions: The chemical (organic or inorganic) is assumed to be released from point, line or area sources into air, deposited onto land and subsequently transported to ground water and surface water. The ATM consists of a steady state Gaussian algorithm. The terrestrial model is a simulation model. The ecological submodels are mechanistic in character.

4. Input and Output: The input data includes monthly wind roses, hourly precipitation, solar radiation, daily maximum and minimum temperatures, soil characteristics, topographic information, surface water characteristics, sediment characteristics, and the physiochemical properties and transformation rates associated with the chemical.

The output consists of plots and tables summarizing the average monthly and annual chemical concentrations in 8 wind sectors, in saturated and unsaturated soil layers, in runoff, out of each reach, and in the stems, leaves, roots and fruits of vegetation.

5. System Resource Requirements: UTM may be run on an IBM 370 series computer or a VAX 11/780 machine. Core storage on an IBM amounts to 540 Kbytes. The model is written FORTRAN IV. Programming experience is helpful in using this model.

6. Applications: The original UTM has been used by the Environmental Sciences Division of Oak Ridge National Laboratory to study the accumulation of trace metals in the soil and biota of two forested ecosystems.

7. Technical Contact:

Joan Lefler (TS-798)
U.S. Environmental Protection Agency
Office of Toxic Substances
401 M Street
Washington, D.C. 20460
COM 202/382-3930 FTS 382-3930

8. References:

Culkowski, W.M., and Patterson, M.R. "A Comprehensive Atmospheric Transport and Diffusion Model." Oak Ridge National Laboratory Report CRNL/NSF/EATC-17 1976.

Patterson, M.R., et al."A User's Manual for the FORTRAN IV Version of The Wisconsin Hydrologic Transport Model. Oak Ridge National Laboratory Report CRNL/NSF/EATC-7, 1974.

Huff, D.D., et al. "TEHM: A Terrestrial Ecosystem Hydrology Model." Oak Ridge National Laboratory Report CRN/NSF/EATC-27, 1977.

URBAN WASTEWATER TOXICS FLOW MODEL (TOXFLO)

1. Model Overview: The Urban Wastewater Toxics Flow Model provides statistical estimation of the generation and fate of toxic pollutants entering into a given municipal sewage treatment system. Quantities computed by the model include flow and concentration values from each controllable industrial discharger and the domestic/commercial sector. It also computes the quality of the influent, effluent, and sludge values from the municipal sewage treatment plant and receiving water quality from the domestic/commercial source. The model can be run to compute either statistical confidence limits for the mean values of these quantities or to predict the frequency distributrion of the daily performance of a system (e.g., how often will water quality criteria be violated.) The model can aid in developing industrial pretreatment programs by indicating which industrial dischargers and toxic pollutants may be problematic under existing levels of treatment and what impact alternative industrial pretreatment/municipal treatment technologies may have in controlling toxic pollutants. The program can be run in a time-sharing mode over an interactive terminal.

2. Functional Capabilities: The model computes a mean, variance, skewness, and kurtosis for flows and concentrations of toxic pollutants at various points within a municipal sewer and sewage treatment system. Depending on the nature of the input data employed, these statistics can be used to estimate confidence intervals for mean values of system performance or to characterize the daily statistical behavior of the system.

3. Basic Assumptions: The model assumes statistical independence between all industrial discharges and between the performance of the municipal treatment plant and the flow in the receiving stream. The frequency distributions of all input quantities must be either normal, log normal, or beta distributed. Serial correlations in time of these quantities is not considered. Municipal treatment plan removal capabilities may be described as a deterministic function of influent concentration coupled to a random error term.

4. Input and Output: Input to the model consists of means and standard deviations for the flow and concentration of each pollutant of interest from each industrial discharger and for the concentrations attributed to domestic/commercial sources. A set of pollutant removal functions and their standard errors is required for the municipal treatment plant. The mean and standard deviation of the receiving stream flow is also needed. There is a possibility that at some future date an internal data base will be added to the model so that the input can be reduced to specifying industrial sub-category types, pretreatment technologies, and municipal treatment technologies.

Standard output from TOXFLO consists of the estimated means of the concentration of each toxic pollutant in the influent, effluent, and sludge of the municipal plant, and of the receiving water. Also, reported is the possibility or frequency with which water quality and sludge quality criteria are violated. The user can request that a more detailed inventory report be printed for a specific pollutant. This report will contain the first four months of the flow, concentration, and mass loading from each discharge source and similar statistics for the concentrations at the municipal treatment plant and in the receiving stream. External to the program, the user may then use this information to assume distribution types for the quantities of interest and then develop confidence limits or determine percentile values.

5. System Resource Requirements: TOXFLO is coded in FORTRAN and is run on an Univac 1100 mainframe. Operation requirements include a background in engineering.

6. Applications: TOXFLO was developed to aid in the planning of industrial pretreatment programs. It can also be used to assist in the analysis of municipal treatment facility discharge permit requirements.

7. Technical Contact

Lewis Rossman
U.S. Environmental Protection Agency
Municipal Environmental Research Laboratory
26 West St. Clair Street
Cincinnati, Ohio 45268
COM 513/684-7636 FTS 684-7636

8. References

A User's Manual is being prepared.

CENTRALIZED TREATMENT OF INDUSTRIAL WASTEWATER

1. Model Overview: The objective of the Centralized Treatment model is to produce an optimal geographic pattern of treatment facilities for industrial wastewater in a metropolitan area. An optimal pattern is one whose annual costs of transporting and treating industrial wastewater is minimal. Treatment facilities may be located at wastewater-producing industrial plants or at one or more candidate sites for centralized treatment. Both capital and operating costs are considered.

The fundamental tradeoff resolved by the model is between the costs of transportation and the economies of scale inherent in centralized treatment.

The model is formulated as a mixed integer program. It is supported by a matrix generator and reports programs.

The model was developed by CENTEC Corporation during 1979 and 1980 in connection with an analysis of centralized treatment as an option for meeting pretreatment regulations published by EPA in 1979. Antecedents include a model for optimizing municipal sludge handling and disposal systems developed by Yakir Hasit in his PhD dissertation at Duke University in 1978, and WRAP, Waste Resource Allocation Program, a model developed for DPA by Mitre Corporation in 1977.

2. Functional Capabilities: The model views the original wastewater workload as 1, 2, or 3 streams emanating from each industrial plant. The 3 stream types are chromium, cyanide, and acid/alkali. Each stream is characterized by a flow rate;

the concentrations of $Cr^{+}3$, $Cr^{+}6$, Cn, Zn, Fe, Ni, Cu, Cd and Pb; through its plant or identification number; and a geographic location. Treatment processes considered are chrome reduction, cyanide oxidation, neutralization/precipitation, flocculation, clarification, thickening, and filtration. Each process may be located at each industrial plant and at each candidate site for central treatment.

Each wastewater source stream is required to undergo full treatment in the sequence neutralization-precipitation, flocculation, clarification, thickening, and filtration. In addition, chrome and cyanide streams must undergo chrome reduction and cyanide destruction, respectively, before entering neutralization/precipitation. Overflows from the clarifier and thickener go to the sanitary sewer. Sludge from the filtration unit goes to a landfill. When wastewater is transported from one site to another, storage tanks with attendant costs are required at each site. Capital and operating costs for each treatment process reflect economies of scale. In addition to wastewater treatment processes, the model considers the economics of wastewater reduction measures applied in the plant production processes to reduce the size of source streams. The model determines the optimal pattern of wastewater reduction, the optimal size of each treatment process at each plant and central site, and transporation flows among sites. Plants and central sites may perform full treatment, partial treatment, or no treatment. A typical problem size is 50-100 plants, 1-3 candidate central sites, and 1-2 landfills. That translates to a typical model size of 4000 constraint equations with 500-1500 integer variables, about half of the latter for representing increasing returns to scale as piecewise linear equations. For mixed integer programs of this size, it is not feasible to run the solution algorithm long enough to prove optimality, but experience indicates that an optimal or near-optimal solution is obtained on the 2nd or 3rd integer-feasible solution when the search criteria are chosen to support that objective.

3. Basic Assumptions: The treatment processes modeled are assumed adequate to meet treatment regulations when properly operated. The performance of clarifiers, thickeners, and filtration units is modeled in terms of fixed efficiencies of solids captured, and fixed ratios of solid to liquid weights in the underflow. Process sizes include a 20% safety factor. Transportation cost is assumed to be a function of payload and distance. It is further assumed that liquid waste is moved in 5500-gallon tank trucks only, filled to capacity. Dewatered sludge is assumed moved in trucks of 30-cubic yard capacity, fully loaded.

Separate capital recovery factors are used for in-plant and central facilities, to permit inclusion of rate-for-return requirements on capital investments by industrial plants. The capital costs of central facilities include a component for site acquisition and construction. Every plant and central site is assumed large enough to accommodate treatment equipment of sizes chosen by the model.

4. Input and Output: The model requires four kinds of input. Technological Data is the cost and performance characterstics of treatment technologies and transporation. With the exception of occasional adjustments to costs, which is provided for in the model via appropriate standard cost indices, this is a reasonably stable set of data that need not be developed anew for each model run. Plant and Source Stream Data is the identification and location, for a region, of each industrial plant whose wastewater requires treatment, and the flow rate and chemical composition of the chrome, cyanide and acid/alkali waste streams at each plant. Input also includes the number of production lines where wastewater reduction has been applied and for which it is feasible. Central Site and Landfill Data is the location of candidate sites for central treatment, and the location of landfills suitable for receiving filtercake

containing precipitated metals. Economic Factors are the interest rates, equipment lifetime, Wholesale Price Index for Industrial Chemicals, Chemical Engineering Plant Cost Index, Chemical Engineering Manpower Cost Index, sewer fee, and landfill fee.

Three principle output reports are produced: plant report, central facility report, and transportation report. The plant and central facility reports show whether a flow reduction or treatment process is present at a site, and, when it is, its size, capital cost, and operating cost. Operating cost is broken out into labor, utilities, and chemicals. When transportation is used, the costs of storage are shown. The transportation report shows the workloads and costs of transporting liquid wastes from plants to central facilities, and transportation among central facilities. The costs of transporting sludge from plants to central facilities and to landfills is also shown. Regional totals are reported by process and resource. Subsidiary outputs include the standard linear programming report of the model solution, and reports of intermediate factors generated during input preparation.

5. System Resource Requirements: The computer program has been written for the Univac 1110 Series using the FMPS and GAMMA language. Additional requirements include short term disk storage for 100 million bytes, and long term storage for 1 million bytes. Any 132 character per line printer may be used. An operator with a background in programming, engineering, and mathematical programming would be helpful.

6. Applications: The model was used by CENTEC Corporation to analyze centralized treatment in the Milwaukee region. The analysis was performed in the project under whose aegis the model was developed.

7. Technical Contact

Alfred Craig
U.S. Environmental Protection Agency
Industrial and Environmental Research Laboratory
Cincinnati, Ohio 45268
COM 513/684-4491 FTS 684-4491

Howard Markham
CENTEC Corporation
11800 Sunrise Valley Drive
Reston, VA 22091
COM 703/471-6300 FTS 471-6300

8. References

CENTEC Corporation, Centralized Treatment Model. User's Manual, August 1980.

CENTEC Corporation, Centralized Waste Treatment Mixed Integer Programming Model -- Milwaukee Results, July 1980.

Yakir Hasit, Optimization of Municipal Sludge Handling and Disposal System, Ph.D. Dissertation at Duke University, Department of Civil Engineering, 1978.

CENTEC Corporation, Centralized Treatment of Metal Finishing Wastes, September 1980.

WRAP, A Model for Regional Solid Waste Management Planning - User's Guide, EPA/530/SW574, U.S. Environmental Protection Agency, February 1977.

COMPUTER PROGRAM FOR CHEMICAL EQUILIBRIA IN AQUEOUS SYSTEMS (REDEQL.DWRD)

1. Model Overview: This program can calculate equilibrium aqueous speciation, saturation states of solids, and dissolved and solid concentrations following precipitation reactions. The program is useful for aquatic toxicology studies, titration experiment modeling (determination of pH or complexation changes), water chemical evaluation for corrosion control treatments, and determination of solubility controls on constituents in natural or drinking waters.

2. Functional Capabilities: The model can include up to 20 metals and 30 ligands at any one time, many of which can be added by the user. The model allows temperature and ionic strength corrections to equilibrium constants. The model allows the user to impose solids in contact with the solution, to prohibit precipitation of supersaturated solids, or to allow precipitation. The program calculates aqueous and solid speciation, interaction intensities and capacities, and can be used to calculate pH. Several other options are noted in References 1 and 2. The accuracy depends on the quality of the thermochemical data, the accuracy of the species chosen to represent the real system, the nearness to equilibrium, and the quality of the anaytical data input.

3. Basic Assumptions: The major assumption is that the system in question is at equilibrium (or can be considered to be in a metastable state that can be treated as equilibrium). Temperature corrections to the equilibrium constants are done by the Van't Hoff relation. Three solids and six complexes are allowed for each metal-ligand pair. Equilibrium constants can contain no more than one decimal place. Mathematical and computational limitations are given in References 1 and 2. Charge balance is not required.

4. Input and Output: A program header card with input and output selections is included with each run. Ten cases can be considered in each run. Concentrations of each metal and ligand can be given in mg/L or - log (molarity). Cards are added for carbon dioxide partial pressure, redox reactions and solids to check saturation indices for precipitation. A test data set is given in Reference 2.

The model can output solid and aqueous speciation in units of "-log (molarity)", and give a table summarizing forms by percentage. Interaction capacities and intensities can be given, and the ionic strength, saturation indices for numerous solids, the pH, and several other parameters can be calculated.

5. System Resource Requirements: This model is coded in FORTRAN G1 and is run on an IBM 370/168 mainframe. It is stored on magnetic tape. It uses any 132 position line printer for output, and a card reader/punch or terminal for input. The manpower needs include a background in water chemistry and ability to input data via cards or terminal.

6. Applications: The model has been used extensively by Drinking Water Research Division, U.S. EPA to determine water quality adjustments to protect asbestos-cement, lead, and galvanized pipe. The program has been used to gain a comprehensive understanding of the naturally-occurring chemical factors involved in preventing the deterioration of asbestos-cement pipe. (see ref 3)

7. Technical Contact

Michael R. Schock
U.S. Environmental Protection Agency
Drinking Water Research Division
26 W. St. Clair Street
Cincinnati, Ohio 45268
513/684-7236

8. References

Ingle, S.E. et al., A User's Guide for FEDEQL.EPA, A Computer Program for Chemical Equilibria in Aqueous Systems, EPA-600/3-78-024 (1978).

Ingle, S.E. et al., REDEQL.EPAK Aqueous Chemical Equilibrium Computer Program. Marine and Freshwater Ecology Branch, Corvallis Environmental Research Laboratory, Corvallis, Oregon (In press, 1980).

Schock, Michael R. and Buelow, R. W., The Behavior of Asbestos-Cement Pipe Under Various Water Quality Conditions, A Progress Report. Part 2 - Theoretical Considerations. Submitted manuscript (1980).

Schock, Michael R., Computer Modeling of Solid Solubilities as a Guide to Treatment Techniques. A paper given at the seminar "Corrosion Control Water Distribution Systems," Cincinnati, Ohio, May 20-22, (1980).

COMPUTER PROGRAM FOR CHEMICAL EQUILIBRIA IN AQUEOUS SYSTEMS (REDEQL. EPAK)

1. Model Overview: The REDEQL.EPAK program computes aqueous equilibria for up to 20 metals and 30 ligands (anions) in a system. The metals and ligands are selected from a list of 35 metals and 59 ligands for which thermodynamic data for complexes and solids have been stored in a data file. More data may be added by the user. The equilibria which the program considers include complexation, precipitation, oxidation-reduction, and pH-dependent phenomena. REDEQL.EPAK is a modification of REDEQL2 which was developed over a number of years at the California Institute of Technology by Morgan, Morel, and McDuff under grants initially from Gulf Oil Corporation, the Environmental Quality Laboratory of Cal Tech, and the Rockefeller Foundation, and, since 1972, under grants from the Environmental Protection Agency.

2. Functional Capabilities: The REDEQL.EPAK program is designed to compute chemical equilibria involving solids, complexes, oxidation-reduction, and mixed solids in an aqueous system. Ionic strength may be calculated or specified and formation constants for solids and complexes are computed from the thermodynamic data for infinite dilution and from ionic strength. Interaction capacities and intensities as described by Morel *et al*. can also be computed.

Up to ten cases of different total concentrations for a set of metals and ligands selected from those available can be treated by the program in one run. A maximum of 20 metals and 30 ligands may be included in any one system considered. The results of the program are the speciation of the metals and ligands in various forms and combinations. A large amount of complexation and solubility data is stored for up to three solids and six complexes for each metal-ligand pair. It is possible to allow for supersaturation with respect to any of the possible solids.

The program may be used with either laboratory, field, or hypothetical input data. The results of the program are based on thermodynamic data, which have been previously measured in less complex systems, applied to the input data. If the formation constant for a solid or complex is not in the thermodynamic data file, that solid or complex will not be predicted to form in the aqueous system being studied, even though it may indeed be present. If a chemical (metal or ligand) present in the system is omitted from the input data for the program, then the results will be in error. If the pH of the system is not known or if the redox potential is not known when oxidation or reduction might occur, then results will be in error. The pH is not required if the chemical form of all species introduced to the system is known.

3. Basic Assumptions: Assumptions and limitations of REDEQL.EPAK follow:

1) The system being modeled is assumed to be at equilibrium. Kinetics of dissolution, precipitation, and oxidation/reduction are not considered.
2) The program does not consider surface effects. Neither the variation of surface properties of solids from bulk properties nor adsorption is included.
3) Errors in analytical or thermodynamic data will be propagated by the program.
4) The ionic strength corrections of equilibrium constants used in the program are not accurate above approximately 0.1 M ionic strength and should not be used above 1.0 M.
5) The program can violate electroneutrality. Nowhere in the computational scheme of the program is the number of

positive charges in a unit volume required to equal the number of negative charges. The "charge" on the equilibrium solution is calculated.

6) Very small concentrations in the output may be inaccurate.
7) Atmospheric concentrations of CO_2 and N_2 must be fixed and cannot vary during a computation except to disappear entirely.
8) No pressure variation is allowed for the thermodynamic data in the program which is given for 25°C and one atmosphere. Temperature data are available for a few thermodynamic constants.
9) At low concentrations, organic matter which is undetected and uncharacterized may strongly affect equilibria.

4. Input and Output: The primary inputs for the program are the total concentrations of metals and ligands in the system, including quantities in solid and gas phases if these are allowed to interact with the aqueous system. Concentration may be in molar units or milligrams/liter. The thermodynamic data file contains thermodynamic data for metals, ligands, solids, complexes, redox reactions, and mixed solids. It presently includes the thermodynamic data for 35 metals and 59 ligands. Input to the program is in card image form.

Output from the model is in the form of computer printouts. Normal output from REDEQL.EPAK include thermodynamic input for verification, input data for the program calculation, case progress for each case, concentration of complexes, speciation of the metals and ligands, primary distribution of metals and ligands, interaction capacities and/or intensities, and error message output.

5. System Resource Requirements: REDEQL.EPAK is available from the EPA IBM computer system in Research Triangle Park, N.C. The

program is run from a load module and requires 200K bytes of core storage. A background in environmental chemistry with familiarity with the model's theory and limitations are helpful.

6. Applications: The model is useful for situations such as 1) mixing compounds together in a beaker of water and predicting what would happen after equilibrium is reached, 2) determining the fate of a chemical introduced into a well-characterized body of water (assuming no further mixing or dilution), 3) predicting removal of chemicals through precipitation under varying conditions of pH, redox potential, and ionic strength, 4) confirming laboratory results for pH or precipitation, 5) predicting pH or metal concentration in aquatic media for biological experiments, and 6) examining mixing and dilution effects in sequential cases with varying initial concentrations.

7. Technical Contact

Don Schultz
U.S. Environmental Protection Agency
Marine and Freshwater Ecology Branch
Corvallis Environmental Research Laboratory
200 S.W. 35th Street
Corvallis, Oregon 97330
COM 503/867-4039 FTS 867-4039

8. References

Ingle, S.E., Schuldt, M.D., and Schults, D.W., "A User's Guide for REDEQL.EPA: A Computer Program for Chemical Equilibria in Aqueous Systems," Corvallis Environmental Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, Corvallis, Oregon, EPA-600/3-78-024, February, 1978.

McDuff, R.E. and Morel, F.M., Technical Report EQ-73-02: Description and Use of the Chemical Equilibrium Program REDEQL2. W.M. Keck Laboratory of Environmental Engineering Science, California Institute of Technology, Pasadena, 1975.

Morel, F. and Morgan, J.J., "A Numerical Method for Computing Equilibria in Aqueous Chemical Systems," Environmental Science Technology, 6:58-57, 1972.

Morel, F., McDuff, R.E., and Morgan, J.J., "Interactions and Chemostasis in Aquatic Chemical Systems - The Role of pH, pE, Solubility and Complexation," in P. C. Singer (ed.), Trace Metals and Metal-Organic Interactions in Natural Waters, Ann Arbor Science Publishers, Ann Arbor, 1973.

Stumm, W. and Morgan, J.J., Aquatic Chemistry, Wiley-Interscience, New York, 1970.

DISSOLVED OXYGEN SAG MODEL (DOSAG-I)

1. Model Overview: DOSAG-I is a mathematical model developed to predict the steady state dissolved oxygen concentrations in streams and canals resulting from a specified set of streamflow, wasteload, and temperature conditions. The model will determine the streamflow required to maintain a specified dissolved oxygen goal and will search the system for available storage to achieve the goal. The model can be used to estimate mean monthly dissolved oxygen levels over a full year. Both carbonaceous and nitrogenous oxygen demands are included,and up to five degrees of treatment for both can be specified. It is one of two programs that the Texas Water Quality Development Board and the EPA has for use in stream quality simulation studies. The other program, QUAL-I, is designed to be used as a complement to DOSAG-I.

2. Functional Capabilities: The purpose of this model is to calculate the biochemical oxygen demand and the minimum dissolved oxygen concentration in a particular stream system. If desired, the minimum dissolved oxygen concentration in the stream system may be checked against a prespecified target level dissolved oxygen concentration. If the minimum dissolved oxygen level is below the target dissolved oxygen level, the program will compute the required amount of flow augmentation to bring the dissolved oxygen level up to the target level in the entire system. The program is designed to be run for varying climatic and hydrologic conditions during a twelve month period. Thus, it is possible to enter up to twelve different temperatures and corresponding discharges to each of the headwaters within the stream system being modeled.

The DOSAG-I model is a one-dimensional, horizontal plane model for streams, rivers, manmade canals and other water conveyance systems. Large impoundments such as reservoirs cannot be considered by this program. A list of restrictions follows:

1) Maximum of 10 headwater stretches
2) Maximum of 20 junctions
3) Maximum of 50 reaches

4) Maximum of 20 stretches
5) Maximum of twelve months of routing for temperature and headwater flows; a minimum of one month must be used
6) Maximum of four dissolved oxygen targets. A minimum of one dissolved oxygen target must be specified. This dissolved oxygen target may be entered as a negative number if no flow augmentation is desired.
7) Maximum of five degrees of treatment for both carbonaceous and nitrogenous wastes; a minimum of one degree of treatment may be specified. If the user does not wish for the degree of treatment calculations to be used in the modeling process, a number less than one should be entered as the treatment factor for both types of wastes.

DOSAG-I has a high sensitivity for residual loads and velocities, and a moderate estimated sensitivity for flow and decay coefficients.

3. Basic Assumptions: The model assumes constant stream velocity throughout each reach and assumes first order decay only. The Streeter-Phelps equation is used to calculate dissolved oxygen concentration, and the computation of atmospheric reaeration is based on the Fickian law of diffusion. A Lagrangian solution technique is used to solve the dissolved oxygen equations.

4. Input and Output: The following are required for input and calibration needs:

1) Reach length
2) Mean velocity
3) Mean discharge
4) Mean depth (per reach)
5) Average reach temperature
6) Residuals discharge inflows
7) Withdrawals and groundwater inflows
8) Residuals inputs (as BOD)
9) Dissolved oxygen concentration in each reach

For verification of the model, streamflows, stream velocity, and observed constituent concentrations throughout the modeled area are required.

Output from the model consists of a tabular printout of the concentration of dissolved oxygen for each reach, BOD (carbonaceous and nitrogenous) at the start and end of each reach, an echo of all input data, and a final summary.

5. System Resource Requirements: DOSAG-I is coded in FORTRAN IV (G level) and requires a digital computer with at least a 27,000 word storage capacity. Data preparation requires 2-6 man-weeks and output analysis takes less than one hour. Actual computation costs run from $1-5. A background in engineering with some basic programming experience is useful.

6. Applications: DOSAG-I was developed by Water Resources Engineers, Inc. and the Texas Water Development Board. The model has been used by the Texas Water Development Board for use in the San Antonio River Basin, and it has been used for a variety of applications by the EPA. DOSAG - I has been replaced in recent years by the more flexible QUAL-II Model.

7. Technical Contact

Tom Barnwell
U.S. Environmental Protection Agency
Center for Water Quality Modeling
College Station Road
Athens, Georgia 30605
COM 404/546-3585 FTS 546-3585

8. References

Finnemore, E.J., Grimsrud, G.P., and Owen, H.J. Evaluation of Water Quality Models: A Management Guide for Planners, prepared for the Environmental Protection Agency, Office of Research and Development, Washington, D.C., under Contract No. 68-01-2641, July 1976.

Texas Water Development Board. "DOSAG-I - Simulation of Water Quality in Streams and Canals: Program Documentation and User's Manual." Report by TWDB Systems Engineering Division, Austin, Texas, 1972.

DYNAMIC ESTUARY MODEL (DEM)

1. Model Overview: The DEM is a "real time" link-node model that simulates the unsteady tidal flow and dispersional characteristics of an estuary. The model can be applied to estuaries in which vertical stratification is either absent or limited to relatively small areas. It can accommodate both conservative and non-conservative constituents. Constituents which have been modeled include salinity, tracer dye, dissolved solids, DO, BOD, total nitrogen, NH_3, NO_3, phosphates, chlorophyll a, and coliform bacteria. Given the necessary kinetics and rates, the model could also treat parameters such as pesticides, heavy metals, and organic compounds. The DEM is often linked to the Tidal Temperature Model (TTM) for heat budgets. Ecological processes such as algal dynamics, nutrient transport, sediment oxygen demand, coliform die-off, and first order kinetics have been expressed in the model. Higher order kinetics are available on some versions.

2. Functional Capabilities: The DEM represents the two-dimensional (lateral and longitudinal) tidal flow pattern, basic transport processes (advection and dispersion), and the accretion or depletion of pollutants within an estuary (provided that vertical stratification is either absent or insignificant). The estuary is represented by a network of channels (or links) and junctions (or nodes). A channel is viewed as a flow conduit with a length, width, time varying depth, time varying velocity, time varying cross-sectional area, and frictional resistance associated with it. A junction acts as a receptacle for mass and volume. It is described by a constant surface area, time varying head, and time varying volume.

The DEM is composed of two separate, but interrelated components. The first component is a hydraulic model which uses a step-forward explicit finite difference scheme to solve the equations of motion and continuity for channels and junctions, respectively. The result is a "dynamic steady-state" solution of the hydrodynamic behavior of the estuary applicable to a specific set of flow inputs and boundary tidal conditions.

The second component, a quality model, is closely tied to the hydraulic model. The quality model and the hydraulic model are referenced to the same network of channels and junctions. The tidally fluctuating velocities, flows, and heads predicted by the hydraulic model are stored on tape or disk and are the basis of the hydraulic inputs to the quality program. Constituents in the quality program are subject to the processes of advection, dispersion (including both eddy diffusion and dispersion due to density currents), biological and/or chemical decay, transfer between water and the atmosphere, and transfer between water and the bottom sediments. A mass balance for each constituent is performed at each junction for each time step. The quality model predicts the dynamic (time varying) constituent concentrations in each junction which result from a specified set of boundary conditions, inflows, waste discharges, and diversions. It is important that the time and space scales used in the DEM approximate as nearly as possible the physical, tidal, and climatic characteristics of the estuary. Special attention should be paid to the correspondence of model network features with existing sampling stations and wastewater inputs.

The DEM is sensitive to (1) the time step in the hydraulic program (stability reasons), (2) net flows, (3) residuals loading rates, (4) frictional resistance coefficient, (5) initial conditions if "real time" solutions are desired, and (6) the specified reaction kinetics and rates.

The Dynamic Estuary Model has been run for networks with as many as 1300 channels and 840 junctions. Some versions have modeled up to 15 constituents.

3. Basic Assumptions: The model assumes that vertical stratification is either absent or limited to relatively small areas, and it does not handle wind stress or tidal flats exposed at low tide. Other hydrodynamic processes assumed negligible include longitudinal density gradients, Coriolis acceleration, and bottom slope. The instantaneous mixing of residuals discharge throughout junctions is also assumed.

4. Input and Output: The DEM requires a large input data base on disk, tape, and/or cards. Parameters which need to be specified include headwater and tributary flows, wastewater flows and loadings, water withdrawals, seaward tidal conditions, channel and junction geometry, bottom roughness of each channel, constituent concentrations at boundaries, and decay rates for non-conservative constituents. Physical data pertaining to channels and junctions can be obtained from navigational charts since direct measurements are seldom available.

The model is capable of producing a wide variety of outputs. Output options available are: (1) maximum and minimum flows, heads, and velocities, as well as net flows, over a tidal cycle for the model network, (2) maximum, minimum, and average constituent concentrations for each junction over a complete tidal cycle (or other specified averaging interval), (3) "slack water" and "snapshot" tables of constituent concentrations at desired time intervals throughout the simulation, and (4) line-printer plots of both spatial and temporal concentration profiles.

5. System Resource Requirements: The DEM is written in FORTRAN IV. The hydraulic component of the model requires 2 files, either on disk or tape. For a network of 129 junctions and 131 channels, the hydraulic program can be run on a digital computer with 130K of main storage. The cost of a 50 hour (4 tidal cycles) hydraulic simulation on an IBM 370/168 is approximately $40. The quality component of DEM requires from 4 to 7 files, depending of the output options desired. A quality program with 6 constituents can be run on a digital computer with 200K to 400K of main storage. The cost of a 1000 hour (80 tidal cycles) quality simulation for 6 constituents and 129 junctions can range from $40 to $75. The DEM requires 5 to 20 manweeks of effort for data preparation and output interpretation. A background in programming and environmental engineering with experience in water quality modeling is useful.

6. Applications: The Dynamic Estuary Model has been used by the EPA for the Pearl Harbor Water Quality Model development project. It was originally developed by the Water Resources Engin-

eers for the Division of Water Supply and Pollution Control of the Public Health Service, and it has been used by the Federal Water Pollution Control Administration (FWPCA) and by the State of California. The DEM was used by the Federal Water Quality Administration (FWQA) for water studies of the San Francisco and San Diego Bay estuaries, and by the EPA for water quality studies of the Delaware and Potomac estuaries. There have been other users and applications of this model.

7. Technical Contacts

Leo J. Clark and Stephen E. Roesch (Potomac application)
U. S. Environmental Protection Agency
Annapolis Field Office
Annapolis Science Center
Annapolis, Maryland 21401
FTS 922-3752 COM 301/224-2740

Robert B. Ambrose (Delaware application)
U. S. Environmental Protection Agency
College Station Road
Athens, Georgia 30605
FTS 250-3546 COM 404/546-3546

8. References

Ambrose, R.B. and Prather, T.L. "Linkage of RECEIV Hydrodynamics with Dynamic Estuary Model Water Quality." From proceedings of the Storm Water Management Model User's Group Meetings, January 19-20, 1981. Department of Civil Engineering. McMaster University, Hamilton, Ontario, Canada.

Ambrose, R.B. and Roesch, S.E. "Dynamic Estuary Model Performance." Journal Environmental Engineering Division ASCE, Paper No. 16847, pp. 51-71, February 1982.

California Water Resources Control Board. "Final Report - San Francisco Bay - Delta Water Quality Control Program." Preliminary Abridged Edition, 1969.

Feigner, K.D., and Harris, H.S. "Documentation Report, FWQA Dynamic Estuary Model." Report to U. S. Department of the Interior, Federal Water Quality Administration, 1970.

Finnemore, E.J., Grimsrud, G.P., and Owen, H.J. "Evaluation of Water Quality Models: A Management Guide for Planners." Report to Environmental Protection Agency, Office of Research and Development, Washington, D.C., 1976.

Genet, L.A., Smith, D.J., and Sonnen, M.B. "Computer Program Documentation for the Dynamic Estuary Model." Report by Water Resources Engineers, Inc., Walnut Creek, California, to U.S. Environmental Protection Agency, Systems Development Branch, Washington, D.C., 1974.

Water Resources Engineers, Inc. "A Hydraulic Water Quality Model of Suisun and San Pablo Bays." Report to U.S. Department of the Interior, Federal Water Pollution Control Administration, Southwest Region.

Water Resources Engineers, Inc. "A Water Quality Model of the Sacramento - San Joaquin Delta." Report by WRE to U.S. Public Health Service, Region IX, 1965.

Water Resources Engineers, Inc. "Computer Program Documentation for the Dynamic Estuary Model." Report by WRE to Florida Department of Pollution Control, Tallahassee, Florida, 1974.

Water Resources Engineers, Inc. "Validation and Sensitivity Analyses of Stream and Estuary Models Applied to Pearl Harbor, Hawaii." Report by WRE, Walnut Creek, California, to U.S. Environmental Protection Agency, Systems Development Branch, Washington, D.C., 1974.

ENHANCED HYDRODYNAMICAL-NUMERICAL MODEL FOR NEAR SHORE PROCESSES (HN)

1. Model Overview: The Hansen type multilayer Hydrodynamical-Numerical (HN) model described by Bauer has been used successfully to study the dynamics of numerous coastal areas. The optimized version of the HN model combines the vertically integrated single layger HN model originally developed by Professor W. Hansen, University of Hamburg, Germany, and the multilayer multiple-open boundary HN model proposed by Hansen and developed by Dr. T. Laevastu.

2. Functional Capabilities: The enhanced HN model simulates near-shore currents and exchange processes. Enhancements to the multilayer Hansen type Hydrodynamical-Numerical model include: non-linear term extension to facilitate small-mesh studies of the near-shore, including river dynamics; layer disappearance extension to enable appropriate procedures in tidal flat and marshy regions, as well as some down/upwelling cases; thermal advection enhancement for treatment of thermal pollution cases by method of moments coupled with heat budget procedures for dynamic plume development experiments; and Monte Carlo diffusion enhancement to deal with dispersion via statistical methods and comparison to the method of moments experiments.

3. Basic Assumptions: The Hydrodynamical-Numerical model is an explicit numerical difference scheme based on leap-frog integration of the two dimensional Eulerian form of the hydrodynamical equations through time to obtain a dynamical boundary-value solution of tidal order. Advection is simulated by the method of moments, a quasi-Lagrangian method which maintains information on the zeroth, first, and second order moments of the concentration in each cell of the grid mesh. In order to introduce the random element for utilization of Monte Carlo methods, the total

velocity for a particular fluid particle is assumed to be composed of a mean flow velocity component and a turbulent flux velocity component. The HN model provides the mean flow velocity and the Monte Carlo scheme provides the turbulent flux velocity. Dispersion is thus modeled by simulating the diffusion process stochastically within the background fluid in motion. The Pedersen-Prahm thermal advection scheme has been chosen since it is a conservative scheme without the pseudo-diffusion of Eulerian difference methods. In order to model the heat budget effects on the thermal discharge as it is transported by the currents throughout the region, the Laevastu thermal techniques were selected.

4. Input and Output: Input to the HN model include grid and mesh size; system geometry, bathymetry, and boundaries; average latitude; Coriolis factor; tidal data; wind values; outfall sources and sinks; storm surge, and river inflow. Control cards and library directives are necessary for the selection of subroutines. Output provided by the model include computer printouts of the input variables and contour plots.

5. System Resource Requirements: Various portions of the HN model are run on Oregon State's CDC 3300 computer, and the Bonneville Power Authority's (BPA) CDC 6500. Experience in environmental modeling and an understanding of the model's theory and limitations are useful for anyone wishing to use the enhanced HN model.

6. Applications: The enhanced HN model has been applied by the EPA to Prudhoe Bay, a section of the coastal area of the Beaufort Sea, Alaska, and the San Onofre outfall in California. The model can be used to evaluate the advection and dispersion of constituents in near shore coastal waters.

7. Technical Contact

Richard J. Callaway
U.S. Environmental Research Laboratory
Corvallis Environmental Research Laboratory
200 Southwest 35th Street
Corvallis, Oregon 97330
FTS 420-4703 COM 503/757-4703

8. References

Bauer, R.A. and Stroud, A.D. Enhanced Hydrodynamical-Numerical Model for Near Shore Processes. In Press. Prepared by Compass Systems, Inc., San Diego, California, for Corvallis Environmental Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, Corvallis, Oregon. EPA Contract 68-03-2225.

Bauer, R.A. Description of the Optimized DPRF Multi-Layer Hydrodynamical-Numerical Model. ENVPREDRSCHFAC Tech. Paper No. 15-74, Environmental Prediction Research Facility, Monterey, California, 1974.

Hansen, W. Hydrodynamical Methods Applied to Oceanographic Problems. In: Proceedings of the Symposium on Mathematical-Hydrodynamical Methods of Physical Oceanography, Institute Fur Meereskunde der Universität Hamburg, Hamburg, West Germany, 1962. pp. 25-34.

Laevastu, T. and Stevens, P., Applications of Numerical-Hydrodynamical Models in Ocean Analysis/Forecasting. FNWC Tech. Note No. 51, Fleet Numerical Weather Central, Monterey, California, 1969.

Laevastu, T. and Rabe, K., A Description of the EPRF Hydrodynamical Models in Ocean Analysis/Forecasting. FNWC Tech. Note No. 51, Fleet Numerical Weather Central, Monterey, California, 1969.

Laevastu, T. A Vertically Integrated Hydrodynamical-Numerical Model (W. Hansen Type), Model Description and Operating/Running Instructions. Part 1 of a series of four reports. ENVPREDRSCHFAC Technical Note No. 2-74, Environmental Prediction Research Facility, Monterey, California, 1974.

Laevastu, T. A Multilayer Hydrodynamical-Numerical Model (W. Hansen Type), Model Description and Operation/Running Instructions. Part 2 of a series of four reports. ENVPREDRSCHFAC Technical Note No. 2-74, Environmental Prediction Research Facility, Monterey, California, 1974.

Laevastu, T. in collaboration with M. Clancy and A. Stroud. Computation of Tides, Currents and Dispersal of Pollutants in Lower Bay and Approaches to New York with Fine and Medium Grid Size Hydrodynamical-Numerical Models. Part 3 of a series of four reports. ENVPREDRSCHFAC Technical Note No. 3-74, Environmental Prediction Research Facility, Monterey, California, 1974.

Laevastu, T. and Callaway,R.,in collaboration with A. Stroud and M. Clancy. Computation of Tides, Currents and Dispersal of Pollutants in New York Bight from Block Island to Atantic City with Large Grid Size, Single and Two Layer Hydrodynamical-Numerical Models. Part 4 of a series of four reports. ENVPREDRSCHFAC Technical Note No. 4-74, Environmental Prediction Research Facility, Monterey, California, 1974.

Laevastu, T. and Hamilton, G.D., Computations of Real-Time Currents Off Southern California With Multilayer Hydrodynamical-Numerical Models with Several Open Boundaries. ENVPREDRSCHFAC Technical Paper No. 10-74.

Pedersen, L.B. and Prahm, L.P., A Method for Numerical Solution of the Advection Equation $\partial C/\partial t=-\underline{V}\cdot\underline{\nabla}C$, Meteorological Institute of Denmark, as submitted to TELLUS, August, 1973.

Laevastu, T. and Harding, J.M., "Numerical Analysis and Forecasting of Surface Air Temperature and Water Vapor Pressure." Journal of Geophysical Research, 79(30):4478-4480, 1974.

Maier-Reimer, E. Numerical Treatment of Horizontal Diffusion and Transport Phenomena in Marine Basins of Large Size, Institüt für Meereskunde der Universität Hamburg, Hamburg, West Germany, as presented at IAMPA/IAPSO Assembly, Melbourne, Australia, January 1974.

Stroud, A. D. and Bauer, R. A. User Guide for the Enhanced Hydrodynamical-Numerical Model. In Press. Prepared by Compass Systems, Inc., San Diego, California, for Corvallis Environmental Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, Corvallis, Oregon, under EPA Contract No. 68-03-2225.

Thompson, R. Numerical Calculation of Turbulent Diffusion. Quart. J. R. Met. Soc. 97(411):93-98, 1971.

Young, Chen-Shyong. Thermal Discharges into the Coastal Waters of Southern California. Southern California Coastal Water Research Project (SCCWRP), Los Angeles, California, 1971.

ESTUARINE WATER QUALITY MODEL (ES001)

1. Model Overview: ES001 is a steady-state, one-dimensional, estuarine water quality model which simulates BOD and DO variations. It was prepared by the EPA to improve upon and document some water quality models developed for the EPA by Hydroscience, Inc., and it is particularly useful for the rapid evaluation of a number of varying estuary and wasteload conditions. Based on the law of conservation of mass, the program is designed to model the BOD-DO deficit system, but it is capable of modeling analogous systems of sequential reactions of two substances having first order kinetics, like that of a nitrogen reaction with ammonia and nitrate. The model is assumed to be at steady state and to be tidally averaged.

2. Functional Capabilities: The program segments the system being modeled into sections within which the various geomorphological, physical, and hydrological parameters of the estuary are constant. For each segment the estuarine steady-state advective-dispersive equation with constant coefficients is defined, the junction points of the segments being boundary points where these parameters can change. Several types of junctions are allowed, including triple junctions, dams, etc., which in combination allow the modeling of numerous types of configurations. A maximum of 100 junctions and 50-100 sections can be accommodated. Each section can have a length of up to 20 miles. Physical processes that can be simulated include: dilution, advection, longitudinal dispersion, temperature effects, and the processes of first order decay and reaeration. The model handles riverine estuaries well, especially when the net velocity is less than one foot per second. The ES001 is sensitive to reaeration coefficients, dispersion coefficients, net flow velocities, and deoxygenation coefficients. A number of output options are provided.

3. Basic Assumptions: ES001 handles only steady-state flows and discharges, and it does not consider flow velocity or quality variations with depth or within stream cross sections. The model assumes only first order kinetics for BOD and DO, and it

utilizes a matrix inversion technique for the solution of simultaneous differential equations which are derived from the Law of conservation of mass.

4. Input and Output: The ES001 requires a large amount of input data in card-image form. Initial input/calibration needs include: estuary cross-sectional data, segment length, water depth, net flow, reservoir outflows, estuary volume, tidal exchange coefficient, dispersion coefficient, constituent concentration for all system inflows, temperatures, benthic oxygen demand, algal photosynthesis, respiration, and other rate coefficients, residual inputs from point sources, uniform waste input, salinities at seaward boundaries, tidal exchange coefficients, and temperature correction factors. Constituent concentrations throughout the system and observed salinity patterns are needed for verification.

Output information provided by the model includes a tabular print-out of the input data, BOD concentration and DO deficits at ten equidistant points per segment, and a number of matrices (DO deficit matrix, BOD matrix, and inverted DO deficit matrix).

5. System Resource Requirements: ES001 is written in FORTRAN IV and may be installed on an IBM System/370 or equivalent. A region size of 245K is utilized by the program, and 2-6 manweeks are needed for data preparation and programming. A background in programming or environmental engineering with familiarity in computerized modeling is useful. A later version of the ES001, the ES002, is designed to run on an IBM 1130 system.

6. Applications: ES001 was developed by Hydroscience, Inc., for the Federal Water Pollution Control Administration (FWPCA) in the Water Quality for the Hudson-Champlain and Metropolitan Coastal Water Pollution Control Project in 1968. The model was one of several simulation programs used to evaluate water quality for the New York Harbor Complex and parts of the Raritan and Hudson Rivers. Since then, ES001 has found other applications.

7. Technical Contacts

George A. Nossa and Laura Livingston
U.S. Environmental Protection Agency
Information Systems Branch 2PM-IS
26 Federal Plaza
New York, New York 10278
FTS 264-9850 COM 212/264-9850

Steven C. Chapra
NOAA Great Lakes Environmental Research Laboratory
2300 Washtenaw Avenue
Ann Arbor, Michigan 48104
FTS 378-2250 COM 313/668-2250

8. References

Chapra, S.C., and Gordimer, S., *Documentation of ES001, A Steady-state, One Dimensional, Estuarine Water Quality Model*, U.S. Environmental Protection Agency, Region II, 26 Federal Plaza, New York, New York, September 1973.

Finnemore, E.J., Grimsrud, G.P., and Owen, H.J., *Evaluation of Water Quality Models: A Management Guide for Planners*, prepared for the Environmental Protection Agency, Office of Research and Development, Washington, D.C., under contract No. 68-01-2641, July 1976.

EXEC/OP VERSION 1.2 (EXEC/OP)

1. Model Overview: EXEC/OP is a FORTRAN computer program that synthesizes municipal wastewater treatment and sludge disposal systems from a specified list of unit treatment process types. It can be thought of as an optimization version of a previously developed treatment system evaluation program known as EXECUTIVE. EXEC/OP will select the combination of unit processes that approximately best meets a stipulated set of criteria on cost, energy, land utilization, a subjective index of system desireability, and effluent quality. It also has the capability to identify up to 40 next-best designs.

2. Functional Capabilities: The model features the following capabilities:

1) The design of the wastewater and sludge treatment sub-system is done in an integrated fashion.

2) Principles of mass balance and reaction kinetics are employed.

3) Nineteen species of pollutants are accounted for.

4) Twenty-two different types of unit processes are included.

5) Eight types of design criteria, plus effluent quality, can be considered.

6) Up to 50 unique process options spread among up to 20 treatment stages, with no more than 10 per stage can be handled.

7) Problems with 15 to 20 thousand design configurations can be solved in several minutes of processing time.

3. Basic Assumptions: EXEC/OP is designed on the basis of steady state mass balance and pollutant transformation relationships. Unit process performance consists of predicting effluent quality, sludge or sidestream quality, equipment sizing, cost, land energy consumption, and production as a function of influent waste quality. A set of design parameters are specified as input by the user. Cost and energy relationships are parameterized on specific design variables and will be accurate to within ± 30 percent. The opimization methodology employed consists of implicit enumeration (a form of integer programming) coupled to a heuristic penalty method that accounts for the impact of return sidestreams from sludge processing.

4. Input and Output: Input specifies the types of unit processes to be considered at each stage of a multi-stage liquid waste treatment train, a secondary sludge treatment train, and a primary or mixed primary-secondary sludge treatment train. A set of input design parameters (e.g., loading rates, kinetic constants, and required effluent quality) is also supplied for each unit process. Unit wage rates and cost indices are used to adjust costs to current prices. Input also includes the quality of the influent waste stream to the system, the required final effluent quality, and a stiulation of the type of design criteria to be used in the optimization (e.g., minimize total cost, minimize energy usage subject to cost not exceeding a certain value, etc.).

Output includes a listing of the unit process choices for each stage of the system in the best design and the M next-best designs, where M is specified by the user. Another output option permits a detailed system performance report to be generated for a given user-specified design.

5. System Resource Requirements: EXEC/OP is coded in FORTRAN IV and is run on an Univac 1100 or PDP 11/70. A background in engineering is useful.

6. Applications: EXEC/OP is an optimization version of a previously EPA developed treatment system evaluation program known as EXECUTIVE. Its purpose is to enable a designer to efficiently synthesize and analyze large numbers of alternative criteria. The program has been used by several wastewater engineering design firms for preparing facilities plans and by universities as a teaching and research aid.

7. Technical Contact

Lewis Rossman
U.S. Environmental Protection Agency
Environmental Research Laboratory
26 West St. Clair Street
Cincinnati, Ohio 45268
COM 513/684-7636 FTS 684-7636

8. References

Rossman, L.A., "Computer Aided Synthesis of Wastewater and Sludge Disposal Systems",: EPA-600/2/79-158, U.S. Environmental Protection Agency, Cincinnati, Ohio, December 1979 (available from NTIS as PB80174220).

Rossman, L.A., "Synthesis of Waste Treatment Systems by Implicit Enumeration", Journal of Water Pollution Control Federation, Vol. 52, No. 1, January 1980.

Rossman, L.A., "EXEC/OP Reference Manual: Version 1.2", EPA-600/2-80-182a, U.S. Environmental Protection Agency, Cincinnati, Ohio, June 1980 (available from NTIS as PB81104176).

Magnetic Tape of EXEC/OP Version 1.2 FORTRAN Source Code, EPA-600/2-80-182b, available from NTIS as PB81104168.

GEORGIA DOSAG (GADOSAG)

1. Model Overview: GADOSAG is a dissolved oxygen model based on the modified Streeter Phelps equation, with options for incremental runoff, an extra non-conservative variable, a converge to set dissolved oxygen routine,and numerous waste inputs.

2. Functional Capabilities: GADOSAG is a steady state, one dimensional, and one stretch model.

3. Basic Assumptions: The model is based on the modified Streeter Phelps equation which predicts dissolved oxygen deficits based on instream concentration of carbonaceous and nitrogenous BOD and their respective reaction rates and the reaeration characteristics of the stream. Inputs are entered by the modeler, and there are no default values.

4. Input and Output: The inputs for this model are: waste treatment facility effluent flow; carbonaceous biological oxygen demand; nitrogenous biological oxygen demand and dissolved oxygen; instream concentrations of CBOD, NBOD, and D.O.; and stream velocity and flow measurements.

The output consists of: dissolved oxygen concentrations along the modeled stream segment, the carbonaceous biological oxygen demand and nitrogenous biological oxygen demand predicted concentrations, and graphs of any of the variables in the model.

5. System Resource Requirements: GADOSAG is coded in BASIC and is run on a HP 9845 or 9831. It uses a 80 character thermal printer. Knowledge of water modeling is useful.

6. Applications: GADOSAG was used by the State of Georgia to set effluent limits for the waste dischargers.

7. Technical Contact

James Greenfield
U.S. Environmental Protection Agency
Water Quality Standards
Atlanta, GA 30365
COM 404/881-4913 FTS 257-2913

8. References

Georgia DOSAGE User's Manual

HYDROLOGICAL SIMULATION PROGRAM--FORTRAN (HSPF)

1. Model Overview: HSPF is a comprehensive package for simulation of watershed hydrology and water quality developed for the U.S. Environmental Protection Agency (EPA). The simulation model uses information such as the time history of rainfall, temperature, and solar radiation; characteristic land use patterns and soil types; and agricultural practices to simulate the processes that occur in a watershed. The result of this simulation is a time history of the quantity and quality of the runoff. Flow rate, sediment load, and nutrient and pesticide concentrations are predicted. The model then takes these results and information about the stream channels in the watershed and simulates the processes that occur in these streams. This part of the simulation produces a time history of water quantity and quality at any point in the watershed--the inflow to a lake, for example. HSPF includes a data management system to process the large amounts of input and output required for the simulations. Computer routines are provided to statistically analyze the data for ease of presentation and interpretation. HSPF can be applied to a wide range of water resource problems. The key attribute that makes it applicable to such a wide variety of water resource problems is its ability to simulate the continuous behavior of time-varying physical processes and provide statistical summaries of the results.

2. Functional Capabilities: HSPF is built on a systematic framework in which a variety of process modules can fit. The system consists of a set of modules arranged in a hierarchical structure that permits the continuous simulation of a comprehensive range of hydrologic and water quality processes. HSPF currently contains three application modules; PERLND,

IMPLND, and RCHRES: and five utility modules; COPY, PLTGEN, DISPLY, DURANL, and GENER. Each of these modules is briefly discussed below.

Module PERLND simulates a pervious land segment with homogeneous hydrologic and climatic characteristics. The simulation of snow accumulation and melt is based on an energy balance approach. Water movement is modeled along three flow paths--overland flow, interflow, and groundwater flow--in the manner of the Stanford Watershed Model. Erosion processes include sediment detachment by rainfall splash and man's influence and transport by overland flow. Scour in rills and gullies is also considered. Water quality constituents may be simulated in the fashion of the NPS model using simple relationships with sediment and water yield or by using the detailed algorithms for pesticides and nutrients as in the ARM model.

Module IMPLND is designed to simulate impervious land segments where little or no infiltration occurs. Algorithms are similar to PERLND except that no water movement occurs by interflow or groundwater flow. Solids are simulated using accumulation and removal relationships in the manner of urban models such as SWMM and STORM. Water quality constituents are simulated using empirical relationships with solids and water yield.

Module RCHRES simulates the processes that occur in a single reach of an open channel or a completely mixed lake. Hydraulic behavior is modeled using the kinematic wave assumption. The outflow of an element may be distributed across several targets that might represent normal outflows, diversions, and multiple gates on a reservoir. Temperature is simulated using a heat balance approach. Sediments are simulated as three size fractions-sand, silt, and clay. Sand transport may be simulated using a power function of velocity, or the Toffaleti or Colby methods. Bed shear stress relationships are used for cohesive sediments (silt and clay.) Both suspended and bed sediment balances are maintained. Conservative and nonconservative constitutents are simulated in a manner that allows maximum user flexibility. The constituent being simulated may be dissolved or associated with any size fraction of sediment. Dissolved constituents may undergo hydrolysis oxidation, pholotysis, volatilization, biodegration or a generalized first-order decay rate may be specified. Daughter products may be simulated in the same fashion as the parent compound. The primary dissolved oxygen and biochemical oxygen demand balances are simulated in the traditional manner, with provisions for decay, settling, benthal sources, reaeration, etc. The primary nitrogen balance is modeled as sequential reactions from ammonia through nitrate. Denitrification is also considered. Both nitrogen and phosphorus are considered in modeling three types of plankton--phytoplankton, zooplankton, and attached algae. Dissolved oxygen is considered in modeling plankton and the nitrogen cycle. Hydrogen ion activity (pH) is calculated considering carbon dioxide, total inorganic carbon, and alkalinity.

HSPF's utility modules are designed to give the user maximum flexibility in managing simulation input and output. COPY is used to manipulate time series. The user can change the form of the time series during the COPY operation. A 5-minute rainfall record may be aggregated to an hourly time interval, for example. The PLTGEN module creates a specially formatted sequential file for later access by a stand-alone plot program. DISPLY takes a time series and summarizes the data in a neatly formatted table. Aggregation of the basic data is also possible. DURANL performs a duration and excursion analysis on a time series and computes some elementarty statistics. It can answer questions like: "How often does dissolved oxygen stay below 4 mg/l for 4 consecutive hours?" The GENER module is used to transform a time series (A) to produce a new series (C) or to combine two time series (A+B) to create a new one (C). For example, this module is useful if one wants to compute the mass outflow of a constituent from the flow and concentration.

3. Basic Assumptions: In a model as comprehensive as HSPF, it is difficult to list all the assumptions made in its development. The watershed hydrologic algorithms generally follow the assumptions made in the Stanford Watershed Model. The agricultural chemical algorithms were derived from the ARM model and the "simple" land surface washoff algorithms are from the NPS model. Both ARM and NPS are described elsewhere in this catalogue. Stream routing uses the kinematic wave approximation and the water quality algorithms use first order kinetics except in the plankton algorithms, where Monod growth kinetics are incorporated. The general quality constituent algorithms used second order kinetics for specific processes and allow kinetic sorption/desorption between dissolved and sediment-associated phases.

4. Input and Output: Data requirements to run HSPF can be quite extensive and depend on the state variables selected for simulation. As a minimum, precipitation and evaporation records are required for simulations. Many parameters can be defaulted but defaults are not provided for the more sensitive, site-specific parameters. System output can be obtained at several levels, from a detailed printout of system state variables and parameter values at every time step to yearly summaries. Printout formats compatible with output interval are provided. An interface file for plotters is provided and a stand-alone program for CALCOMP plotters is available.

5. System Resource Requirements: HSPF requires a FORTRAN compiler that supports direct access I/O. Twelve (12) external files are required. The system requires 128K bytes of instruction and data storage on virtual memory machines, or about 250K with extensive overlaying on overlay-type machines. The system was developed on a Hewlett-Packard 3000 minicomputer and has been used on IBM 370 series computer. It has also been installed on PRIME, HARRIS, and Burroughs minicomputers, and on Univac and CDC mainframes.

Because of its comprehensive nature, HSPF requires individuals with several different backgrounds to implement it. As a minimum, an implementation team should consist of a systems programmer, a hydrologist, and a water quality expert. Personnel requirements for data preparation and output interpretation will vary with the system being modeled.

6. Applications: Although HSPF is a relatively new product, having been publically released by EPA in April 1980, it has undergone some testing through applications to inhouse projects by the developer (Hydrocomp, Inc.). It has also been used in projects sponsored by EPA. Some of these applications are described below.

In a 208 study, a prototype of the HSPF system was applied to the Occoquan River Basin by the Northern Virginia Planning District Commission. The Occoquan Basin Computer Model consists of 15 sub-basins (39 mi^2 average) linked by a network consisting of 12 stream channels and 3 reservoirs and was based on a linkage of the NPS model and HSP. Considerable effort went into data collection to calibrate the runoff and stream quality models, resulting in one of the better general nonpoint source data bases. The model was used to project long-term receiving water quality impacts of existing and future (year 2005) land use patterns and to compare the benefits of alternative "best management practice" (BMP) levels. The HSPF software was tested largely using the simulations of the Occoquan basin as a reference.

One of the early applications of HSPF was in a hydropower study for the Dominican Republic. Hydropower is a major source of electricity in this developing country, which is experiencing an 11% annual increase in demand. Twenty potential hydropower sites were identified and 10 potential network configurations were hypothesized. The analysis procedure consisted of the generation of 99 years of synthetic hourly precipitation, calculation of land surface runoff, and calculation of natural stream flow at 21 sites. Power generation was simulated by routing the streamflow through the 10 different hydropower configurations. The time series for depth of flow (head) and flow rate were then analyzed using the GENER module to estimate the most efficient configuration.

Another water resources study using HSPF has been conducted in the Clinton River Basin, Michigan. The purpose of the study was to evaluate a proposed Corps of Engineers floodway, estimate the impact of developing wet lands, investigate better lake operating procedures, and simulate the effect of retention ponds. The basin is located north of Detroit and lies in Macomb and Oakland counties. It is largely urban in the south and agricultural in the north. The HSPF network consisted of four land segments for each of nine rain gauges and 128 channel reaches in six sub-basins. The model was calibrated on a ten-year record (1965-1975). Simulated annual peak flows were then compared with 14 USGS stream gauges for the period 1927-1975. The longer time period was then used to evaluate water resource management options.

EPA is currently applying HSPF, through a contractor, merged with the Chemical Migration and Risk Assessment (CMRA) methodology, to demonstrate its application as a planning tool for the evaluation of agricultural BMP's. This demonstration is being done at two scales--the 20 mi^2 Four Mile Creek watershed in east central Iowa and the 1200 mi^2 Iowa River Basin above Coralville Reservoir. The small scale demonstration serves as a calibration site for scale-up to the larger basin. A number of potential BMP implementation scenarios will be investigated relative to their impact on water quality. Different scenarios will focus on a mix of structural, non-structural, and input-management related practices. Schemes aimed at receiving water quality targets for pesticides, phosphorus, and nitrates will be simulated.

HPSF is also being used by the State of Nebraska to investigate the effect of groundwater pumping for agriculture in the Big Blue Basin. The University of Nebraska is using the system as a data management tool for the Dee Creek Research Watershed. A project sponsored through the University of North Dakota is using HSPF to investigate the effect on wildlife habitat of proposed lake drainage in the basin of the Red River of the North.

An ongoing maintenance and training program is sponsored by the center for Water Quality Modeling.

7. Technical Contact

Thomas O. Barnwell, Jr.
U.S. Environmental Protection Agency
Center for Water Quality Modeling
Environmental Research Laboratory
College Station Road
Athens, Ga. 30613
FTS 250-3585   404/546-3585

Hydrocomp, Inc.
201 San Antonio Circle
Mountain View, CA 94046
COM 415/948-3919

8. References

Anderson, E.A. "Development and Testing of Snow Pack Energy Balance Equations." Water Resources Research, 4(1):19-37, 1968.

Barnwell, T.O. and Johanson, R.C. "HSPF: A Comprehensive Package for Simulation of Watershed Hydrology and Water Quality." Presented at: Nonpoint Pollution Control: Tools and Techniques for the Future, Gettysburg, PA, June 1980.

Crawford, N.H. and Donigian, A.S. Jr. Pesticide Transport and Runoff Model for Agricultural Lands. EPA-600/2-74-013. Environmental Research Laboratory, Athens, GA 30613, 1973.

Crawford, N.H. and Lindsey, R.K. Digital Simulation in Hydrology: Stanford Watershed Model IV. Stanford Univ. Tech. Rep. No. 39, Stanford Univ., Palo Alto, CA, 1966.

Donigian, A.S., Jr., Beyerlain, D.C., Davis, H.H., Jr., and Crawford, N. H. Agricultural Runoff Management (ARM) Model Version II: Refinement and Testing. EPA-600/3-77-098. Environmental Research Laboratory, Athens, GA 30613, 1977.

Donigian, A.S., Jr. and Crawford, N. H. Modeling Pesticides and Nutrients on Agricultural Lands. EPA-600/2-76-043. Environmental Research Laboratory, Athens, GA 30613, 1976.

Donigian, A.S., Jr. and Crawford, N.H. Modeling Nonpoint Pollution From The Land Surface. EPA-600/3-76-083. Environmental Research Laboratory, Athens, GA 30613, 1976.

Donigian, A.S., Jr. and Crawford, N.H. Simulation of Nutrient Loadings in Surface Runoff with the NPS Model. EPA-600/3-77-065. Environmental Research Laboratory, Athens, GA 30613, 1977.

Donigian, A.S., Jr. and Crawford, N.H. User's Manual for the Nonpoint Source (NPS) Model. Unpublished Report. Environmental Research Laboratory, Athens, GA 30613, 1979.

Donigian, A.S., Jr. and Crawford, N.H. User's Manual for Agricultural Runoff Management (ARM) Model. EPA-600/3-78-080. Environmental Research Laboratory, Athens, GA 30613, August 1978.

Grimsrud, G.P., Franz, D.D., Johanson, R.C., Crawford, N.H. Executive Summary for the Hydrologic Simulation Program -- FORTRAN (HSPF). In Press. Environmental Research Laboratory, Athens, GA 30613, 1980.

Hydrocomp, Inc. Hydrocomp Simulation Programming: Operations Manual, 2nd Edition, Hydrocomp, Inc., Palo Alto, CA, 1969.

Johanson, R.C., Imhoff, J.C., and Davis, H.H. User's Manual for the Hydrologic Simulation Program -- FORTRAN (HSPF). Environmental Research Laboratory, Athens, GA 30613, 1980.

Leytham, K. M. and Johanson, R.C. Watershed Erosion and Sediment Transport Model. EPA-600/3-79-028. Environmental Research Laboratory, Athens, GA 30613, 1979.

Negev, M. A Sediment Model on a Digital Computer. Stanford Univ. Tech. Rep. No. 76. Stanford Univ., Palo Alto, CA, 1967.

LAKE-I ECOLOGIC MODEL (LAKE-I)

1. Model Overview: The LAKE-I Ecologic Model is a water quality model used in the evaluation of fresh water lakes. It is a two-dimensional, time variable model that includes temperature, nitrogen and phosphorous in a three layer system. The model simulates the ecological process of photosynthesis, growth, decay, and respiration. It considers algal-nutrient relationships, algal-zooplankton dynamics, and relatively simple higher consumer relationships. The principle driving forces of the Lake-I model include vertical dispersion between layers, lake inflows-lake outflow, and inflows split proportionally between layers. The model was originally developed by Thomann, DiToro, Winfield, and O'Connor at Manhatten College, Bronx, New York for the EPA Large Lakes Research Station in Grosse Ile, Michigan.

2. Functional Capabilities: LAKE-I is a stratified three layer system. The epilimnion extends from the surface to a 17 meter depth, the hypolimnion occurs between 17 meters and a 90 meter depth. A sediment layer is included as a material sink. The physical transport of advection and dispersion are considered only for exchange between the epilimnion and hypolimnion. A thermocline is established by setting vertical dispersion between layers to near zero, and seasonal overturns are simulated by variable mixing rates.

Constituents modeled by LAKE-I include nitrogen,(organic N, ammonia, and nitrate), phosphorous (organic P and ortho P), organic carbon (zooplankton), and phytoplankton chlorophyll. The Lake-I model adequately represents nutrients and phytoplankton in an open lake. A later revision, LAKE-III can handle horizontal transport and simulations of phytoplankton, zooplankton, and nutrients. Model coefficients include variable vertical mixing rates, phytoplankton settling velocity, nutrient half-saturated values and herbivore grazing rates.

3. Basic Assumptions: The LAKE-I Ecologic Model is based on deterministic assumptions and is numerically integrated by the finite difference method. Mixed horizontal dimensions with vertical gradients are assumed.

4. Input and Output: Input to the model for initial set-up and calibration include: segment depth; average segment water temperature variations with time, solar radiation and photo-period; water clarity, nutrient inputs as mass loadings (mass/unit time) or boundary conditions (mass/unit volume); and initial conditions for phytoplankton, zooplankton, and consumer biomass. Model date requirements for verification incorporate observed concentrations of chlorophyll a, primary production (mg C/M^2/day), total zooplankton carbon, bottom deposition rate (mg C/M^2/year), total phosphorous, orthophosphorous, and total Kjedahl nitrogen, ammonia, and nitrate.

Output from LAKE-I include the phytoplankton chlorophyll for a one year simulation, nutrient pools, and zooplankton biomass. Output at 0.5 day time steps are also possible. Output formats are given as printed tables which can yield digital overplots, or as tape outputs which can yield 3-D plots or visual projections.

5. System Resource Requirements: The model is coded and operational in FORTRAN IV, and it is currently being run on a CDC 6600 system. Newer versions of the model will be available on IBM and DEC equipment. Total CPU time is equal to 30 CPU seconds for a one year simulation, with an actual execution time of 7 CPU seconds. At least 8-16 annual runs are needed to reach a steady state.

Manpower needs include a computer programmer or an environmental engineer with programming experience. Some experience in water quality models based on FORTRAN IV is helpful. Data collection programs would involve limnologists, biologists, and chemists.

6. Applications: The LAKE-I Model has been used by the EPA at its Large Lakes Research Station at Grosse Ile, Michigan for the modeling of Lake Ontario as part of its Great Lakes Modeling Program and has been applied to Saginaw Bay.

7. Technical Contact

William L Richardson
U.S. Environmental Protection Agency
Large Lakes Research Station
9311 Groh Road
Grosse Ile, Michigan 48138
FTS 226-7811 COM 313/226-7811

8. References

Thomann, R.V., DiToro, D.M., Winfield, R.P., and O'Connor, D.J., Mathematical Modeling of Phytoplankton in Lake Ontario, Vol. 1: Model Development and Verification. U.S. Environmental Protection Agency, Corvallis, Oregon, 660/3-75-005, March 1975.

Thomann, R.V., Winfield, R.P., DiToro, D.M., and O'Connor, D.J. Mathematical Modeling of Phytoplankton in Lake Ontario, Vol. 2: Simulations Using LAKE-I Model. U.S. Environmental Protection Agency, Duluth, Minnesota. In press.

LEVEL III - RECEIVING WATER QUALITY MODELING

FOR URBAN STORMWATER MANAGEMENT

1. Model Overview: Level III-Receiving is a simplified continuous receiving water quality model that can be used as a planning guide to permit preliminary screening of area wide wastewater treatment strategies. The model was designed to interface with hourly continuous urban catchment hydrologic simulation models such as STORM or SWMM (both described elsewhere in this catalogue). A large number of urban pollution control alternatives can be simulated and evaluated in terms of their impact on receiving water quality. Evaluation is accomplished by evaluating either classical dissolved oxygen sag curves or cumulative frequency curves of dissolved oxygen concentration. The model computes a minimum interevent time to define statistically independent storm events.

2. Functional Capabilities: Level III - Receiving can accommodate a large number of inflow combinations of receiving water flow, dry-weather flow, and wet-weather flow. Oxygen concentration is considered the key to the quality of natural water bodies, although it is certainly not the only viable water quality indicator. Urban runoff quantity and quality must be computed with a model like STORM or SWMM. Receiving water effects are computed using a simplified modeling approach. Advective and dispersive transport is modeled. The dissolved oxygen balance includes carbonaceous BOD and reaeration. Nitrogenous oxygen demand is neglected.

3. Basic Assumptions: Assumptions typical of models limited to interim planning are made, including:

1) Temporal steady-state conditions prevail, i.e., all system parameters and inputs (other than stormwater inputs) are constant with respect to time.

2) Natural system parameters (such as flow, velocity, depth, deoxygenation and reaeration rates, and longitudinal dispersion) are spatially constant throughout each time step.

3) All waste inflows occur at one point.

4) The effects of various natural biological processes (algal photosynthesis and respiration, benthal stabilization) are incorporated into a background quality reflected by an upstream D.O. deficit. Any benthic buildup is incorporated in the BOD decay rate.

5) Waste treatment facilities operate at constant efficiency, independent of hydraulic and organic loadings, for the entire period of simulation.

4. Input and Output: Program input consists of STORM/SWMM output and data cards organized into 5 major card groups. Card group I controls the execution of the three major subprograms. Card group II controls the autocorrelation analysis of hydrologic time series. Card group III contains input data common to both the wet weather and dry weather flow models. Card group IV contains the wet weather flow model input. Card group V is specific to the dry-weather flow model.

Program output consists of tables and plots describing the system response, including correlograms of time series, frequency histograms or cumulative frequency curves of D.O. concentrations, and tables of D.O. concentrations at specified locations.

5. System Resource Requirements: The program has been tested on the IBM 370/165 and Amdahl 470-V6/II computers. It may be compiled under either the G or H-level FORTRAN compilers. Core requirements are approximately 100K bytes on the IBM 370/165. Typical costs for the example problem described in the documentation range from $5 to $25 for one year of simulation.

6. Applications: Level-III Receiving may be applied to the surface drainage of most urban catchments. There is no limitation to the size of catchment or number of storm events modeled (other than computer time and costs). Data requirements are common to engineering analysis of nonpoints source problems and complete instructions on data preparation are provided. Field measurements are necessary to calibrate model parameters and verify predicted values. The methodology is not applicable to systems requiring multi-dimensional transient analysis. Complex water quality conditions such as eutrophication, non-linear kinetic interactions, sedimentation, and sediment exchange are not represented.

7. Technical Contacts

Richard Field
U.S. Environmental Protection Agency
Storm and Combined Sewer Section
Edison, N.J. 08837
FTS 340-6674 COM 201/321-6674

Dr. Miguel A. Medina
Department of Civil Engineering
Duke University
Durham, N.C. 27706
919/684-2434

8. References

Medina, M.A., Jr., Level-III: Receiving Water Quality Modeling for Urban Stormwater Management. EPA-600/2-79-100. U.S. Environmental Protection Agency, Cincinnati, OH 45268, 1979.

M.I.T. TRANSIENT WATER QUALITY NETWORK MODEL

1. Model Overview: The M.I.T. Transient Water Quality Network Model is a one-dimensional, real-time, nitrogen cycle model which can be used for nitrogen-limited, aerobic estuarine systems. The model solves one-dimensional continuity and momentum equations to generate the temporal and spatial variations in the tidal discharges and elevations. This information is used in the solution of the conservation of mass equations for the water quality variables, which include salinity, temperature, carbonaceous BOD, nitrogen cycle variables, DO, and fecal coliform. The model combines the work of many investigators and has undergone a great deal of modification. It was originally developed at the Ralph M. Parsons Laboratory for Water Resources and Hydrodynamics at the Massachusetts Institute of Technology, and its broadest application has been the St. Lawrence River and Estuary. The model is intended to be used in engineering decisions regarding the degree of eutrophication due to distributed and point source loadings in estuaries.

2. Functional Capabilities: The model was developed for aerobic estuarine ecosystems and includes seven storage variables and twelve transformations of nitrogen between those variables. The storage variables include: 1) N_1, Ammonia-N, 2) N_2, Nitrite-N, 3) N_3, Nitrate-N, 4) N_4, Phytoplankton-N, 5) N_5, Zooplankton-N, 6) N_6, Particulate Organic-N, and 7) N_7, Dissolved Organic-N. The transformations include: 1) nitrification, 2) uptake of inorganic nitrogen by phytoplankton, 3) grazing of herbivores, 4) ammonia regeneration in living cells, 5) release of organic matter from living cells, 6) natural death of living organisms, and 7) ammonification of organic nitrogen. The user can specify a branching and or looping network of channels called reaches where each reach can be of variable cross-section along its longitudinal axis. Storage volumes are provided for along the reach and any number of concentrated or distributed water quality loadings can be specified along each reach. The flow regime can be that of an estuarine system with an unsteady tidal elevation driving the

circulation at the ocean boundaries in combination with the upstream flow.

For subcritical flow, three possible boundary conditions can be specified, and these are: 1) the Discharge Q, 2) the surface elevation Z, and 3) a relationship between Z and Q. The model can simulate control structures within the network itself instead of only at the boundaries, and the user is permitted to specify a boundary condition at the upstream side of the control structure. Three possible boundary conditions (concentration, dispersion flux, and total flux) and a special ocean boundary procedure are provided.

3. Basic Assumptions: The M.I.T. Transient Water Quality Network Model defines the geometry of the water body along a particular reach by interpolation between the cross-sectional data submitted by the user. The model pays strict adherence to the mass conservation principle as applied to the element nitrogen, and its ecosystem model is coupled with a real-time hydrodynamic transport system as opposed to a tidal-average or slack-tide approximation. The structure of the model was formulated such that the level of complexity would not be too complex to the point of diminishing returns, nor too simplified to the point where rate-governing parameters must be determined by curve fitting the available field data. Carbonaceous BOD is handled as a first order decaying substance in the classical manner.

4. Input and Output: Input data is divided into nine groups. Card Group A includes information regarding solution options. Here it is stipulated which solutions (hydraulic and water quality) will be executed and which water quality parameters will be modeled. Time parameters stipulating the duration of the run and the time step of integration, and the network topology (identification and sequence of reaches) is also provided.

Card Group B provides the geometric information (i.e., the physical properties of the channel), and the computational mesh spacing and initial conditions required for the hydraulic solution. This group is repeated for each reach as given in Group A.

Card Group C provides values of rate coefficients for those water quality parameters being modeled. The coefficients may be specified for the entire network or may be specified for each individual reach. If the user does not wish to specify values, the program will automatically use default values. In this card group, the computational mesh spacing for water quality calculations and initial conditions for water quality parameters are also specified.

Card Group D describes the location, magnitude and quality of any lateral inflows being considered. Lateral inflows are considered for both the hydraulic and water quality solutions. Card Group E describes the same information for any injections (e.g. sewerage treatment plant or waste heat discharge) of water quality parameters. Injections are considered only in the water quality solution. For hydraulic purposes they are considered passive, that is, they have no effect on the flow field in the receiving water. Card Group F stipulates the hydraulic boundary conditions to be applied at each node.

Card Group G allows the user to selectively view output from the hydraulic solution. Card Group H stipulates the water quality boundary conditions to be applied at each node in the network, and Card Group I allows the user to selectively view output for the water quality solution. The sequence of the input cards is important to note. Certain card groups (D,E,F, G,H,I) for particular cases must be repeated several times corresponding to the number of periods for which the solution is executed.

The large volume of numerical information generated by the computer is conveniently represented in graphical form. A plotting program is available for use on an incremental drum plotter. The output for the hydraulic solution can be requested in two forms: 1) a hydrograph which displays the parameters at a given mesh point as a function of time, and 2) a hydraulic profile which displays the parameters at a given time as a function of distance. The hydraulic parameters displayed are surface elevation, depth, discharge, and velocity. Output for the water quality solution also may be displayed in two forms: 1) water quality graphs, i.e., parameters as a function of time, and 2) water quality profiles, i.e., parameters as a function of distance. Special features permit the user to plot several variables on the same frame and also to plot user-supplied data points as special symbols.

5. System Resource Requirements: The model is coded in FORTRAN IV (H), and storage space allocation is as follows: 256K for compilation, 226K for execution, and 92K for the plotting program. The program utilizes 4,445 source statements (not counting comments) and consists of 47 routines. The time required for data preparation and output interpretation will vary with the system being modeled. A background in environmental engineering with experience in computer modeling is useful.

6. Applications: The model has had a number of applications, the broadest application being to the St. Lawrence River and Estuary, a study sponsored by the Canadian Departments of the Environment and Transport and Quebec Service de Protection de l'Environment and Ministere des Richesses Naturelles. Thatcher, Pearson, and Mayor-Mora have described the application to both riverine and estuarine portions of the St. Lawrence River from Cornwall to Montmagny, a distance of 275 miles. The need for a published user's manual was recognized by the National Environmental Research Center, U.S. EPA, Corvallis, Oregon, and their support has enabled documentation of the model at this stage of its development. The EPA has used the model for test purposes.

7. Technical Contacts

Richard J. Callaway
U.S. Environmental Protection Agency
Corvallis Environmental Research Laboratory
200 S.W. 35th Street
Corvallis, Oregon 20036
FTS 420-4703 COM 503/757-4703

8. References

Chow, V.T., Open Channel Hydraulics, McGraw Hill, N.Y., 1959.

Dailey, J.E. and Harleman, D.R.F., "Numerical Model for the Prediction of Transient Water Quality in Estuary Networks", Technical Report No. 158, R.M. Parsons Laboratory for Water Resources and Hydrodynamics, Department of Civil Engineering, M.I.T., October 1972.

Gunaratnum, D.J. and Perkins, F.E., "Numerical Solution of Unsteady Flows in Open Channels", Technical Report No. 127, R.M. Parsons Laboratory for Water Resources and Hydrodynamics, Department of Civil Engineering, M.I.T., July 1970.

Harleman, D.R.F., Brocard, D.N. Najarian, T.O., "A Predictive Model for Transient Temperature Distributions in Unsteady Flows", Technical Report No. 175, R.M. Parsons Laboratory for Water Resources and Hydrodynamics, Department of Civil Engineering, M.I.T., November 1973.

Harleman, D.R.F. and Thatcher, M.L., "Longitudinal Dispersion and Unsteady Salinity Intrusion in Estuaries", La Houille Blanche/No. 1/2 - 1974.

Harleman, D.R.F., Dailey, J.E., Thatcher, M.L., Najarian, T.O., Brocard, D.N., and Ferrara, R.A. "User's Manual for the M.I.T. Transient Water Quality Network Model", Report for U.S. Environmental Protection Agency, Office of Research and Development, Corvallis Environmental Research Laboratory, Corvallis, Oregon. U.S. EPA Publication EPA-600/3-77-010, January 1977.

Henderson, F.M. Open Channel Flow, MacMillan Co. N.Y., 1966.

Larsen, P.A., "Hydraulic Roughness of Ice Covers", JHD, ASCE 99, HYI, January 1973.

Najarian, T.O. and Harleman, D.R.F., "A Real Time Model of Nitrogen-Cycle Dynamics in an Estuarine System", Technical Report No. 204, R.M. Parsons Laboratory for Water Resources and Hydrodynamics, Department of Civil Engineering, M.I.T., July 1975.

Surveyer, Nenniger & Chenevert, Inc. and Carrier, Trottier, Aubin, "Hydrodynamic and Water Quality Simulation Model: Cornwall-Montmagny Section", Report to Department of Environment, Canada, March 1973.

Surveyer, Nenniger & Chenevert, Inc. and Carrier, Trottier, Aubin; (in French) "Hydrodynamic and Water Quality Simulation Model: Cornwall-Montmagny Section", Report to Service de Protection de l'Environment Quebec, March 1974.

Thatcher, M.L. and Harleman, D.R.F., "Mathematical Model for the Prediction of Unsteady Salinity Intrusion in Estuaries", Technical Report No. 144, R.M. Parsons Laboratory for Water Resources and Hydrodynamics, Department of Civil Engineering, M.I.T., February 1972.

Thatcher, M.L., Pearson, H.W., and Mayor-Mora, R.E., "Application of a Dynamic Network Model to Hydraulic and Water Quality Studies of the St. Lawrence River", 2nd Annual Symposium of the Waterways, Harbours and Coastal Engineering Division, ASCE, San Francisco, September 1975.

MULTI-SEGMENT COMPREHENSIVE LAKE ECOSYSTEM ANALYZER FOR ENVIRONMENTAL RESOURCES (MINI. CLEANER)

1. Model Overview: The Multi-Segment Comprehensive Lake Ecosystem Analyzer for Environmental Resources (MINI. CLEANER) is one of the more biologically realistic aquatic ecosystem models. Because of the attention to general process-level constructs, the model is appropriate for application to diverse types of lakes and reservoirs and is capable of addressing many environmental problems.

The model represents over 30 man-years of development by a multidisciplinary team. The precursor, CLEANER, was formulated by 25 investigators from several institutions under the aegis of the International Biological Program, Eastern Deciduous Forest Biome. The model is structured to simulate up to 20 biotic and 20 abiotic state-variables in each of 10 spatial segments simultaneously. Current development includes adaptation to coastal environments and coupling to a model for bioaccumulation of toxic substances. MINI. CLEANER was developed by Dr. Richard A. Park of the Center for Ecological Modeling, Rensselaer Polytechnic Institute, Troy, New York, for the U.S. Environmental Protection Agency.

2. Functional Capabilities: MINI. CLEANER is an ecological model capable of addressing environmental problems such as nutrient enrichment, thermal pollution, siltation, imponndment, and fish removal. The model can simulate a variety of biotic variables, including four types of phytoplankton (two with internal storage of nitrogen and phosphorous); up to four types of submerged aquatic vegetation (macrophytes); five types of zooplankton; two or more types of fish with as many as four life stages; two kinds of bottom-dwelling animals (zoobenthos); and three groups of decomposers (bacteria and fungi). An equal number of abiotic variables can be simulated, including seven types of dissolved organic matter; four types of particulate organic matter; five types of inorganic

nutrients in the water column and sediments; and four compartments for dissolved oxygen and inorganic carbon. This potential complexity is seldom fully utilized, however. Normal applications require a subset of perhaps 20 state-variables. The model has been run with as few as two dynamic state-variables. Several external variables and all the biotic state variables can be used as loadings. External variables include water temperature, temperature and discharge rate of inflowing water, wind speed, light, dissolved inorganic nitrogen, orthophosphate, dissolved silica, dissolved organic material, and particulate organic material.

As a user-oriented model, MINI. CLEANER features a machine-independent namelist editor that enables the user to list and make changes in parameter values while running the model; to plot state-variable concentrations, rates for various processes, and loadings to the model; and to transform the state-variable values into "environmental perception" characteristics such as turbidity, fish catch, or concentrations of noxious algae.

Multiple segments can be simulated, each having different physical-chemical and biotic characteristics. Movement of materials across the boundaries of the segments is specified by a linking language. The movement can either be intersegmental or be treated as a loss from the system, as specified by the user.

The loadings of nutrients, temperature, and light can be perturbed using the editing capability of MINI. CLEANER to set at the perturbation parameters. The perturbations can be either additive or multiplicative, and either constant or as a pulse of user-specified duration and timing.

An algorithm has been developed to facilitate analysis of the sensitivity of MINI. CLEANER to changes in values of parameters and driving variables. Using a random number generator, values with a normal or uniform distribution are used to vary loadings or parameters within a specified range. The simulation is repeated a given number of times with different perturbations, and the results are summarized. The parameters are perturbed at the beginning of each simulation; the loadings are perturbed at each step.

3. Basic Assumptions: The realism of MINI. CLEANER is achieved by disaggregation of state-variables and by use of detailed process equations. Adaptive constructs are used for light and temperature response in phytoplankton. These constructs have permitted application to a wide range of lakes without changing parameters.

Unlike most ecosystem models, MINI. CLEANER can treat phytoplankton growth as a function of stored nutrients. This uncoupling of growth and external nutrient concentrations has resulted in more realistic simulations with avoidance of the time lags between modeled and observed phytoplankton peaks that are a persistent problem with many models.

Likewise, process-level realism in simulating zooplankton has been achieved by recognizing variations in modes of food consumptions. In some zooplankton the rate of consumption is independent of the concentration of food; in others a minimum food level is necessary before feeding will occur. The rate of consumption follows saturation kinetics.

In order to use MINI. CLEANER in studying bioaccumulation of toxic substances, the fish compartments have been disaggregated to represent age classes. At the time of promotion, all, or some fraction, of the fish in one age class is transferred to the next age class at a rate that follows a normal distribution. The shedding of gonadal products (and associated pesticides) by adults is handled in the same manner.

By modeling decomposers explicitly, more realistic simulations of decomposition have been obtained. This is particularly important in representing the differential degradation of different types of organic material (including oil spills), the cycling of nutrients, and--through the production of microbial biomass--formulation of a high-quality food source for detritus feeding animals.

Phosphorus, silicon, carbon and soluble inorganic nitrogen are the only nutrients that can be limiting. The temperature, nutrient, and biomass are considered to be uniformly distributed in a segment.

4. Input and Output: The data required to calibrate and use the model fall into several categories:

1) Driving Variables - a time-series of data for the period of the simulation (which may be from a few days to years), including water temperature, incident radiation, loadings of dissolved and particulates, organic matter, biomass, and nutrients.
2) Site Constants - average water depth and light extinction coefficient.
3) Initial Conditions - for all variables.
4) Parameter Values - a default set of values for the extensive parameter list may be used or values that are known may be input.
5) Calibration Data - observed values for some state variables are necessay to fine-tune the model.
6) Pertubations and Sensitivity Analysis - sensitivity to changes in parameters and driving variables may be examined using a built-in algorithm.

All of the input data and parameter values used can be output as well as the state variables simulated. A plotting routine is available.

5. System Resource Requirements: MINI. CLEANER requires approximately 64K bytes of core. Ten files are required for operation of the program, plus an additional number of files equal to the number of segments being simulated (up to 10 segments). Execution times depend on the complexity and length of the simulation. The model is coded in FORTRAN IV. Current work includes adaptation to minicomputers. The model has run on the PDP 11/03 computer although execution times are excessive. It should be adaptable to any 16-bit scientific minicomputer with 64K bytes of memory.

6. Applications: The model has been calibrated and verified with data from a number of lakes of diverse types. It was originally applied to Lake George, New York. Subsequent versions have been calibrated for Lock Leven, Scotland; Slapy Reservoir, Czechoslovakia; Balaton Lake, Hungary; Lakes d'Endine and Mergozzo, Italy; Lake Esrum, Denmark; Lake Paijanne, Finland; and DeGray Reservoir, Arkansas. A version that incorporates all the latest improvements, including storage of internal nutrients in phytoplankton, has been calibrated for subalpine Ovre Heimdalsvatn, Norway, and verified with data from Vorderer Finstertaler See, Austria, without changing parameter values. With only minor changes, it gives reasonable results for Lake Mergozzo, a mesotrophic, stratified lake.

Because of the complexity of the program, application requires a sophisticated user familiar with ecologic and computer modeling concepts. A short residency at Rensselaer Polytechnic Institute is recommended for those who wish to use the model.

7. Technical Contacts.

Thomas O. Barnwell, Jr.
U.S. Environmental Protection Agency
Environmental Research Laboratory
College Station Road
Athens, Georgia 30605
FTS 250-3585 COM 404/546-3585

Dr. Richard A. Park
Center for Ecologic Modeling
Rensselaer Polytechnic Institute
Troy, New York 12181
COM 518/270-6494

8. References

Bloomfield, J. A., Park, R. A., Scavia, D., and Zahorcak, D. S. "Aquatic Modeling in the Eastern Deciduous Forest Biome, U.S. International Biological Program." In: Middlebrooks, E. J., D. H. Falkenborg, and T. E. Maloney (Editors), Modeling the Eutrophication Process, Utah State University, Logan, Utah, pp. 139-158, 1973.

Clesceri, L.S., Park, R. A., and Bloomfield, J. A. "General Model of Microbial Growth and Decomposition in Aquatic Ecosystems." Appl. Environ. Microbiol., 33(5):1047-1058, 1977.

deCaprariis, P., Park, R. A., Haimes, R., Albanese, J., Collins, C., Desormeau, Groden, T., Leung, D., and Youngberg, B. "Utility of the Complex Ecosystem Model MS.CLEANER." In: Proceedings of the International Conference on Cybernetics and Society, pp. 87-89, 1977.

Desormeau, C. J. "Mathematical Modeling of Phytoplankton Kinetics with Application to Two Alpine Lakes." Report #4, Center for Ecological Modeling, Rensselaer Polytechnic Institute, Troy, New York, 21 pp., 1978.

Groden, T. W. "Modeling Temperature and Light Adaptation of Phytoplankton." Report #2, Center for Ecological Model, Rensselaer Polytechnic Institute, Troy, New York, 17 pp., 1977.

Leung, D. K. "Modeling the Bioaccumulation of Pesticides in Fish." Report #5, Center for Ecological Model, Rensselaer Polytechnic Institute, Troy, New York, 18 pp., 1978.

Leung, D. K., Park, R. A., Desormeau, C. J., and Albanese, J. "MS.CLEANER: An Overview." In: Proceedings of Pittsburg Modeling and Simulation Conference, Pittsburg, Pennsylvania, 1978.

Park, R. A. "Theoretical Implications of Models of Aquatic Systems." Presented at AAAS, Biological Sciences Meeting, New York, New York 1975.

Park, R. A. "A Model for Simulating Lake Ecosystems." Report #3, Center for Ecological Modling, Rensselaer Polytechnic Institute, Troy, New York, 19pp., 1978.

Park, R. A. "Predicting the Impact of Man on Lake Ecosystems." (Abstract) In: Biro, P. (Editor), Human Effects on Life in Fresh Water, Hungarian Academy of Sciences, Tihany, Hungary, 1977.

Park, R. A., O'Neil, R. V., Bloomfield, J. A., Shugart, H. H., Booth, R. S., Goldstein, R. A., Mankin, J. B., Koonce, J. F., Scavia, D., Adams, M. S., Clesceri, L. S., Colon, E. M., Dettmann, E. H., Hoopes, J., Huff, D. D., Katz, S., Kitchell, J. F., Kohberger, R. G., LaRow, E. J., McNaught, D. C., Peterson, J., Titus, J., Weiler, P. R., Wilkinson, J. W., Zahorcak, C. S. "A Generalized Model for Simulating Lake Ecosystems." Simulation, 23 (2): 33-50, 1974.

Park, R. A., Scavia, D., and Clesceri, N. L."CLEANER, the Lake George Model." In: Russell, C. S. (Editor), Ecological Modeling of a Resource Management Framework. Resources for the Future, Inc., Washington, D. C. pp. 49-82, 1975.

Park, R. A., Grodin, T. W., and Desormeau, C. J."Modifications to the Model CLEANER Requiring Further Research." In: Scavia, D. and A. Robertson (Editors), Perspectives on Aquatic Ecosystem Modeling, Ann Arbor Science Publishers, Inc., 1978.

Park. R. A., Collins, C. D., Leung, D. K., Boylen, C. W., Albanese, J., deCaprariis, P., and Forstner, H. "The Aquatic Ecosystem Model MS.CLEANER." Center for Ecologic Modeling, Rensselaer Polytechnic Institute, Troy, New York, 1978.

Scavia, D., Boylen, C. W., Sheldon, R. B., and Park, R. V."The Formulation of a Generalized Model for Simulating Aquatic Macrophyte Production." Fresh Water Institute Report #75-6, Rensselaer Polytechnic Institute, Troy, New York, 1975.

Scavia, D. and Park, R. A. "Documentation of Selected Constructs and Parameter Values in the Aquatic Model CLEANER." Ecol. Mod., 2(1): 33-58, 1976.

Youngberg, R. A. "Application of the Aquatic Model CLEANER to a Stratified Reservoir System." Report #1, Center for Ecological Modeling, Rensselaer Polytechnic Institute, Troy, New York, 22 pp., 1977.

NATIONAL RESIDUALS DISCHARGE INVENTORY (NRDI)

1. Model Overview: The NRDI is a quantitative assessment of residual generation and discharges (total suspended solids, BOD, nitrogen, phosphorous, and nutrients) and of residual reduction technology costs in each of 3,111 counties or county approximations in the contiguous U.S. Data for industrial, municipal, urban runoff, and non-irrigated agriculture sources are available for each county. However, the data are not displayed at the county level, but rather are aggregated for purposes of analysis by the Water Resources Council's 99 aggregated sub-areas (ASAs), the 18 Water Resource Regions (WRRs) and by the nation. The model was developed under the auspices of the National Academy of Sciences, Washington, D.C.

2. Functional Capabilities: The NRDI is a series of FORTRAN programs and data bases which provide estimates of current and projected discharges of wastes (total suspended solids, BOD, nitrogen and phosphorus) to surface waters, and capital and operation and maintenance costs of treatment facilities. The model estimates pollutant discharges and costs by industrial or municipal facility for approximately 40,000 point-source discharges, and by county for urban storm runoff and non-irrigated agriculture. These detailed estimates are then aggregated as desired. Discharges and costs are estimated for conditions of (1) no control, (2) controls in place in 1973, (3) 1977 standards, and (4) 1983 standards.

The NRDI allows for an evaluation of policy alternatives to the uniform application of residual reduction technologies to legislatively defined (P.L. 92-500) point sources. These policies reflect alternatives where in a given ASA or WRR, achievement of the 1983 effluent limitations would not make a significant improvement in total residual reductions and ambient water quality, and where a given level of residual reduction could be achieved at a lower cost without the uniform application of residual reduction technology to point sources.

3. Basic Assumptions: The model consists of (1) inventories of production and consumption activities which generate and discharge residuals, (2) a system for analyzing the effects of increased industrial and population growth, (3) an index of potential water quality changes, and (4) residual discharge reduction policies which include the BPT/ST (best practicable control technology currently available/secondary treatment) and BAT/BPWTT (best available technology economically achievable/best practicable waste treatment technology) technology goals in the Federal Water Pollution Control Act (P.L. 92-500).

For point-source discharges, discharge and cost estimates are based on simulation of specific end-of-pipe technologies for discharge reduction. Discharge conditions in 1973 as well as 1977 and 1983 standards are estimated for specific industrial facilities or industry subgroups. For municipal facilities, the 1974 EPA Needs Survey is used. For urban runoff, required treatment is estimated based on work done for the National Commission on Water Quality. For non-irrigated agriculture, information from the 1967 Conservation Needs Inventory is used.

4. Input and Output: Major inputs to the NRDI include the EPA Needs Survey, the Conservation Needs Inventory, County Business Patterns, City-County Data Book, and Census data. A detailed industrial source inventory was developed for the model. Thus, the model contains information on identifiable point and areal source residual generating activities which cover most waterborne residual generating activities. Information included about these activities, where appropriate and available, are location of activity, measures of production (physical output, employees, land area, or population), type of production process, and current residual reduction technologies being used.

Outputs are produced by county-aggregate unit, and source category or subcategory. A variety of alternative policies can be selected for solution in the NRDI. These policies include both uniform and non-uniform abatement policies and can simulate controls on areal as well as point sources. The outputs from each policy alternative are: residual generation, residual discharge, abatement costs, and residuals dilution index. The basic policies used to date are discussed below:

1) No control - This policy estimates residuals discharge if no control technology is used.
2) 1973 controls - This policy estimates discharge and costs based on control technology in place in 1973.
3) BPT/ST - This policy estimates effects of the 1977 standards of the P.L. 92-500: Best Practicable Treatment for industry and Secondary Treatment for municipalities.
4) BAT/BPWTT - This policy estimates the effects of the 1983 standards for industry and secondary treatment for municipalities supplemented with tertiary facilities when requested in the EPA Needs Survey.
5) BAT/BPWTT+ - This policy is identical to (3) for industrial sources but includes filtration for all municipalities not requesting treatment more stringent than secondary in the EPA Needs Survey.
6) Non-irrigated agricultural control - Costs and residual implications of implementing practices outlined in the 1967 Conservation Needs Inventory are included.
7) Urban storm control - Costs and residual implications of one of five urban storm control strategies (combined, separate storm, and unsewered) is simulated.
8) Ocean discharges - Effects of discharge and costs for ocean counties are excluded. This function is used to simulate lower levels of treatment for ocean discharges based on using a specified set of counties.
9) New source performance standards - In this policy, residual discharges and costs for industrial growth are based on new source performance standards (approximated by BAT).
10) Limited technology - Simulation of stringent effluent limitation policies can be limited to ASA with relatively bad water quality.
11) Cost effective strategy - This policy used data on cost

per quantity of residuals removed to identify cost-effective solutions in each ASA.

Combinations of these policy components can be combined in a single run if desired.

5. System Resource Requirements: All programs are written in FORTRAN for an IBM 360/370 system. Programs run in 200K bytes or less. A full run can be made for under $100. Manpower requirements include a computer programmer or an environmental engineer with experience in environmental modeling.

6. Applications: NRDI results have been used for the following:

1) The book: Water Pollution Control: Assessing the Impacts and Costs of Environmental Standards (Praeger, 1977).
2) The report: The National Residuals Discharge Inventory (National Academy of Sciences, 1976).
3) The 1976 Annual Report of the Council on Environmental Quality.
4) The Water Resources Council's 1975 National Assessment.
5) The National Commission on Water Quality's Environmental Technical report.

7. Technical Contact

Ralph A. Luken
U.S. Environmental Protection Agency
Economic Analysis Division
401 M. Street, S.W.
Washington, D.C. 20460
FTS 382-5475 COM 202/382-5475

8. References

Black, Crow, and Eidsness, Study and Assessment of Capabilities and Costs of Technology for Control of Pollutant Discharges from Urban Runoff, NCWQ Contract, November 1975.

Luken, Basta, and Pechan, The National Residuals Discharge Inventory, National Research Council, Washington, D.C., January 1976.

Midwest Research Institute, Cost and Effectiveness of Control of Pollution from Selected Non-point Sources, NCWQ Contract, July 1975.

Pechan, E.H., and Luken, R.A., "A Water Residuals Inventory for National Policy Analysis.", Proceedings of the Conference on Environmental Modeling and Simulation, U.S. EPA publication EPA 600/9-76-016, July 1976.

U.S. Department of Commerce, Bureau of the Census, 1972 County Business Patterns, Washington, D.C.

U.S. Department of Commerce, Bureau of the Census, 1972 Census of Manufacturers, Water Use in Manufacturing, Washington, D.C.

U.S. Department of Commerce, Bureau of the Census, 1972 City County Data Book, Washington, D.C.

U.S. Environmental Protection Agency, Joint State-EPA Survey of Needs for Municipal Waste Water Treatment Facilities, computer tape, March 1975.

U.S. Water Resources Council, 1972 OBERS Projections, April 1974.

Wharton Econometric Forecasting Associates, Wharton Econometric Forecasting Estimates, Mark IV, Solution of March 4, 1975.

OUTFALL PLUME MODEL (PLUME)

1. Model Overview: PLUME is a computer program which can be used to evaluate coastal waters, lakes, or estuaries under consideration as disposal sites. It is designed to evaluate and/or predict the length of outfall needed to adequately dilute a proposed discharge in order to provide compliance with water quality standards. The model was developed by the U.S. EPA Environmental Research Laboratory in Corvallis, Oregon, and it has been used by the San Juan Field Office of the U.S. EPA to aid in the location and analysis of ocean outfalls.

2. Functional Capabilities: PLUME simulates the three dimensional (two dimensions in the horizontal plane and one dimension in the vertical plane) initial dilution of the effluent plume of residuals in lakes, coastal waters, and estuaries. Some of the factors which can be evaluated by PLUME include the effects of onshore currents, tides, density and salinity gradients, ambient surface and hypolimnetic velocities, the initial jet velocity, the quantity of discharge, the slope of the ocean bottom, and the rates of coliform die-off in the vicinity of outfall locations. The model simulates a stratified aquatic environment, and up to 50 layers are permitted.

PLUME is sensitive to discharged fluid density and flow rate, and also to extent of stratification. The model is also sensitive to the physical features of the outfall - the diameter of openings, the number of ports, and the port depth.

3. Basic Assumptions: The model simulates the behavior of a buoyant, round effluent plume being discharged into a non-flowing water body where it considers the density differences between freshwater (with residuals) and saltwater masses. The model does not simulate the transport of discharged residuals by mechanisms other than mixing and dilution of fluids with different densities, and it assumes no water flow other than the plume-induced movement. A steady-state, stratified aquatic environment is assumed.

4. Input and Output: Input to the PLUME program should be in card-image form. Initial setup/calibration needs include: (1) water temperature profile (with depth), (2) salinity or density profile (with depth), (3) effluent flow rate, (4) effluent density, and (5) the outfall features such as the port diameter, number of discharge points, depth of discharge points, and the angle of the discharge points to the horizontal plane. The initial constituent concentration throughout the plume is needed for verification.

The model provides a tabular printout of the following output information: (1) labeled input values, (2) constituent dilution along the plume centerline, and (3) the depth at which the plume stabilizes.

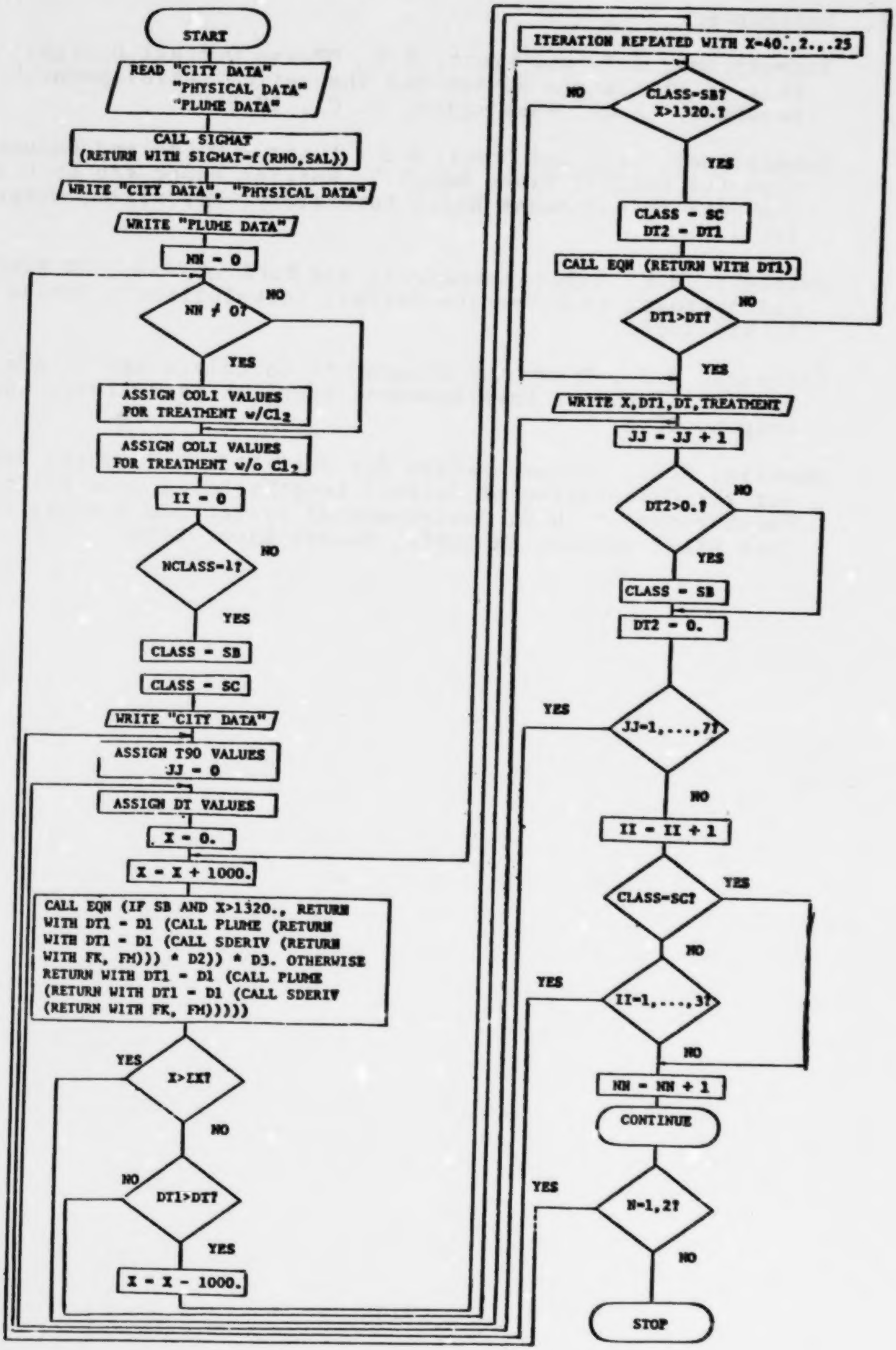
5. System Resource Requirements: PLUME is coded in FORTRAN IV and requires a FORTRAN IV compiler. The program is compatible with the IBM 370/155 and requires 10,000 words of core storage. Up to one man-week is necessary for data preparation. and only one or two man-hours for output interpretation. A background in computer programming or ~~in~~ hydraulics engineering with environmental modeling experience is useful.

6. Applications: Outfall plume was developed by the U.S. EPA Environmental Research Laboratory in Corvallis, Oregon, and the model has been used by the San Juan Field Office of the U.S. EPA to aid in the location and analysis of ocean outfalls. PLUME has also found other applications and other users.

7. Technical Contacts

George A. Nossa and Laura Livingston
U.S. Environmental Protection Agency
Information Systems Branch 2PM-IS
26 Federal Plaza
New York, New York 10278
FTS 264-9850 COM 212/264-9850

Richard J. Callaway
U.S. Environmental Protection Agency
Corvallis Environmental Research Laboratory
200 SW 35th Street
Corvallis, Oregon 97330
FTS 420-4703 COM 503/757-4703


START
READ "CITY DATA"
"PHYSICAL DATA"
"PLUME DATA"
CALL SIGMAT
(RETURN WITH SIGMAT=f(RHO,SAL))
WRITE "CITY DATA", "PHYSICAL DATA"
WRITE "PLUME DATA"
NN = 0
NN ≠ 0?
NO
YES
ASSIGN COLI VALUES
FOR TREATMENT w/Cl₂
ASSIGN COLI VALUES
FOR TREATMENT w/o Cl₂
II = 0
NCLASS=1?
NO
YES
CLASS = SB
CLASS = SC
WRITE "CITY DATA"
ASSIGN T90 VALUES
JJ = 0
ASSIGN DT VALUES
X = 0.
X = X + 1000.
CALL EQN (IF SB AND X>1320., RETURN
WITH DT1 = D1 (CALL PLUME (RETURN
WITH DT1 = D1 (CALL SDERIV (RETURN
WITH FK, FM))) * D2)) * D3. OTHERWISE
RETURN WITH DT1 = D1 (CALL PLUME
(RETURN WITH DT1 = D1 (CALL SDERIV
(RETURN WITH FK, FM)))))
YES
X>IX?
NO
NO
DT1>DT?
YES
X = X - 1000.
ITERATION REPEATED WITH X=40.,2.,.25
NO
CLASS=SB?
X>1320.?
YES
CLASS = SC
DT2 = DT1
CALL EQN (RETURN WITH DT1)
DT1>DT?
NO
YES
WRITE X,DT1,DT,TREATMENT
JJ = JJ + 1
DT2>0.?
NO
YES
CLASS = SB
DT2 = 0.
YES
JJ=1,...,7?
NO
II = II + 1
CLASS=SC?
YES
NO
YES
II=1,...,3?
NO
NN = NN + 1
CONTINUE
YES
N=1,2?
NO
STOP

Flowchart for OUTFALL PLUME

8. References

Baumgartner, D.J. and Trent, D.S., "Ocean Outfall Design: Part I, Literature Review and Theoretical Development." Report by FWPCA, Washington, D. C., 1970.

Baumgartner, D.J. and Trent, D.S., "User's Guide and Documentation for Outfall Plume Model." Working Paper #80 by U.S. EPA Pacific Northwest Water Laboratory, Corvallis, Oregon, 1971.

Burchett, M.E., Tchobanglous, G., and Burdoin, A.J., "A Practical Approach to Submarine Outfall Calculations". Public Works. 5, 95, 1967.

Callaway, R.J., "Computer Program to Calculate ERF". EPA Pacific Northwest Environmental Research Laboratory, Corvallis, Oregon, 1973.

Guthrie, D.L., "Documentation for Outfall: A Computer Program for the Calculation of Outfall Lengths Based upon Dilution Requirements." U.S. Environmental Protection Agency, San Juan Field Office, Santurce, Puerto Rico, 1975.

RECEIVING WATER MODEL (DIURNAL)

1. Model Overview: DIURNAL is a one-dimensional (horizational plane) receiving water quality model. The model represents the physical processes of advection and dilution and simulates receiving water quality changes in dissolved oxygen. Coupled chemical reactions can be simulated, and dissolved oxygen, CBOD and NOD can be modeled. The primary function of DIURNAL is to predict the diurnal fluctuations during periodic steady-state conditions. The model was developed by Hydroscience, Inc. of Westwood, New Jersey.

2. Functional Capabilities: The DIURNAL model can be applied to streams and rivers under one-dimensional, steady-state conditions. It allows a stream length to be analyzed with any number of functional segments; the number being dependent only on the frequency of in-stream characteristics changes, waste discharge (or withdrawal) locations, and accuracy desired. Each segment, likewise, can be divided into any number of functional elements, again dependent on desired accuracy. The following effects have not been included in the solution; the time variation of flow, the time variation of the temperature and wasterwater discharges and the effect of dispersion. The sources and sinks of dissolved oxygen considered in the model include reaeration, biochemical oxygen demand, nitrogenous oxygen demand, benthic oxygen demand, photosynthesis, and respiration. The model is best used in conjunction with a steady state water quality model to fix all parameters except respiration and photosynthesis. DIURNAL would then be used to determine these two parameters on a periodic steady-state basis.

3. Basic Assumptions: The solution analysis is an extension of the technique based on the continuity equation for dissolved oxygen which includes the diurnal time-variable effect of photosynthetic oxygen production. The analysis considers the temporal as well as spatial distributions. The periodic extension of the photosynthetic oxygen production is expressed as a Fourier series.

4. Input and Output: Input information is basically of three types; initial conditions definition, individual segment characteristics definition and discharger information. Initial conditions data include system description (number of sections, element length, river mile at the head of the system) and quality description (upstream BOD, upstream NBOD, and Fourier coefficients of upstream DO). The individual segment data include the following; section length, velocity, temperature, reaeration rate, and decay rates (carbonaceous and nitrogenous). Other information includes bottom demand, hours of daylight, maximum photosynthetic rate, respiration, time of sunrise, stream flow, and segment elevation. Discharger information includes, DO, flow, BOD, and NOD. Segment characteristics and discharger information is repeated for each segment modeled.

DIURNAL produces a tabular printout of section parameters and dissolved oxygen response. The section parameters include; length, velocity, temperature, flow, reaeration, and decay rate, benthic rates and photosynthesis and respiration rates. The DO response table includes hourly dissolved oxygen values, for 24 hours, for the beginning and the end of the segment, and any intermediate point designated by the print interval.

5. System Resource Requirements: DIURNAL is coded in FORTRAN IV (G) and can be run on a digital computer with a 40,000 word core storage capability; FORTRAN IV (G) compiler. Application of the model results in minimal costs, in the range of \$1 - \$2 per run, including on the number of segments. Approximately 1-man week is required for model setup and data preparation. Initial runs on a companion model is necessary to establish appropriate velocities and rates. A background in environmental engineering with a programming background is helpful.

6. Applications: DIURNAL can be used on any stream where it is assumed that the primary cause of the diurnal variation of the dissolved oxygen is the algal oxygen production.

7. Technical Contact

Thomas Henry
U.S. Environmental Protection Agency
Region III Water Division
Curtis Building
6th and Walnut Street
Philadelphia, Pa. 19106
FTS 597-8048 COM 215/597-8048

8. References

Di Toro, Dominic, and O'Connor, Donald J. "Photosynthesis and Oxygen Balance in Streams", Journal of the Sanitary Engineering Division, ASCE, April 1970, PP 547-571.

RECEIVING WATER MODEL (RECEIV-II)

1. Model Overview: RECEIV-II is a two dimensional receiving water model for streams, rivers, estuaries, lakes, and reservoirs. The model represents the physical processes of advection, dispersion, and dilution, and it can simulate flows, tidal movements, and water surface changes in a link-node network. Coupled and non-coupled chemical reactions can be simulated, and dissolved oxygen, BOD, coliforms, nutrients, salinity, conservative constituents, chlorophyll a, and non-conservative constituents with first order decay can be modeled. RECEIV-II is a modification of the receiving water module of the Storm Water Management Model (SWMM) developed by Water Resources Engineers, Metcalf and Eddy, and the University of Florida.

2. Functional Capabilities: The RECEIV-II model can be applied to streams, rivers, estuaries, lakes, and reservoirs. Dynamic conditions are represented, and an option is available for steady state conditions. The model is two dimensional and permits up to 225 channels and up to 100 junctions in a link-node network. RECEIV-II can simulate estuarine flats at low tide by varying cross-sectional area, and it can handle multiple tidal inlets, upstream dams, and unsteady inflows such as residual discharges, storm runoff, and tides. The physical processes of advection, dispersion, and dilution are represented. Chemical processes represented include coupled and uncoupled reactions, DO, BOD, coliforms, nutrients, salinity, conservative constituents, chlorophyll a, NH_3, NO_2, and non-conservative constituents with first order decay. The model does not consider stratified systems, but it does consider ocean tide exchange at a single input point. RECEIV-II lacks the ability to simulate temperature, but it does consider wind stress and direct rainfall inputs. The model is

sensitive to quality time step size and decay coefficients. Lateral and vertical velocity variation within the channels can be broken-up laterally for a two dimensional effect.

3. Basic Assumptions: The model is based on deterministic assumptions and uses a finite difference methods as a solution technique. RECEIV-II assumes instantaneous mixing throughout each junction, and it uses a two dimensional channel network to simulate two dimensional flow and transport.

4. Input and Output: Input to the model for initial setup and calibration includes: constant headwater inflow rates; flow rate for each inflow (discharge, tributary, etc.) or withdrawal; tidal cycles and heights at the seaward boundary; widths and depths of each channel; initial flow velocities and water surface elevations throughout the system; initial constituent concentrations throughout the system; residual loading rates from discharges, tributaries, and headwaters; tidal exchange coefficient; meteorological data (wind speed, rainfall, and daily solar radiation); and first order decay rates for constituents. Input for verification of the model includes: net flow and velocities for each channel; data record of constituent concentration throughout the modeled system; and salinity data to establish concentration inputs at the seaward boundary.

The model produces a tabular printout of: maximum, minimum, and net flows for each tidal cycle; maximum, minimum, and average constituent concentrations in each channel at specified time intervals; and depth at each junction at specified time intervals. Hydrodynamic output (especially channel velocities) can be written onto magnetic tape or disk.

5. System Resource Requirements: RECEIV-II is coded in

FORTRAN IV (G), and can be run on a digital computer with 400K bytes of core storage,a Fortran IV (G) compiler, and two magnetic tapes or disks. Application of the hydrodynamic module costs between $15-$100 per run, and application of the quality module ranges from $10-$50 per simulation run. The actual expenses of using RECEIV-II is dependent upon the extent of discretization, time step size, and length of simulation. Depending on the model complexity, 1-5 man-months are needed for model set-up and data preparation. Several manhours are necessary for output analysis. A background in computer programming and hydraulics engineering with a basic programming background are useful. The model may be obtained from the Planning Assistance Branch of the Environmental Protection Agency.

6. Applications: RECEIV-II can be linked to the terrestrial flow routing module of the Storm Water Management Model (SWMM), or it can be utilized by itself to simulate dynamic conditions. RECEIV-II has been used by the U.S. Army Corps of Engineers, and it is currently being utilized by the EPA in Regions III and IV.

7. Technical Contact

Tom Barnwell
Center For Water Quality Modeling
U.S. Environmental Protection Agency
Environmental Research Laboratory
College Station Road
Athens, GA 30613
FTS 250-3585 COM 404 / 546-3585

8. References

Metcalf and Eddy, Inc., University of Florida, and Water Resources Engineers, Inc., Storm Water Management Model, Volumes 1-4, Report to U.S. Environmental Protectinn Agency, Washington, D.C., 1971 (EPA Report No. 11024DOC).

"Stormwater Management Model User's Guide, Version II",
For the U.S. Environmental Protection Agency - Report No.
EPA-670/2-75-017, March 1975.

RECEIVING WATER QUALITY MODEL (RWQM)

1. Model Overview: The Receiving Water Quality Model (RWQM) was developed by Resource Analysis, Inc. for the U.S. Army Corps of Engineers 'Hydrologic Engineering Center to interface with STORM (Storage Treatment Overflow Runoff Model). RWQM (HEC, 1979), when linked with the time history of storm and dry-weather flows generated by STORM, provides the capability to predict the impact and land surface runoff on stream water quality.

2. Functional Capability: RWQM simulates the one-dimensional transport and transformation of six water quality parameters (temperature, DO, carbonaceous BOD, nitrogenous BOD, orthophosphate, coliforms) in freshwater streams.

3. Basic Assumption: RWQM simulates time-varying hydraulic and water quality conditions by utilizing the law of mass conservation for water and pollutant volumes. Stream routing uses the kinematic wave assumption. Water quality parameters are modeled using first order kinetics.

4. Input and Output: RWQM input is on cards and tape files. Input consists of, for each stream reach: Stream reach and segmentation, simulation controls, I/O controls, percentile curve limits and location, atmospheric temperature input, monthly stream equilibrium temperature, monthly heat transfer rate coefficients, reaction rate coefficients, reaction rate temperature modification bases, gauged baseflow information,

stream hydraulics information, boundary conditions, tributary flows, point sources, nonpoint sources, volumetric sources and sinks, STORM runoff and dry weather flow, combined sewer overflows, storage releases and treated outflow, and initial conditions.

RWQM offers a wide range of statistical output to both summarize and provide "snapshots" of simulated instream conditions. Long term average, maximum and minimum pollutant concentrations, temperatures, and flows are tabulated; and frequency (percentile) curves can be computed. In addition, parameter profiles can be printed for any day or "pollutagraphs" for chosen locations.

5. System Resource Requirements: The RWQM is designed to operate on a high speed digital computer having a FORTRAN IV compiler. It has been tested on both an IBM 370 and a CDC 7600. It makes extensive use of computer tape and/or disk storage for temporary and permanent saving of input data and simulation output.

6. Applications: The RWQM can be used in conjunction with the STORM land runoff model. It has been applied to Pennypack Creek (Abbott and Willey, 1979) in the Philadelphia area.

Computer program documentation costs $4 from the Hydrologic Engineering Center, Davis, California. The source deck can be obtained from HEC for $120.

7. Technical Contact

R. G. Willey
Hydrologic Engineering Center
Corps of Engineers
609 Second St.
Davis, CA 95616
FTS 448-3292   COM 916/440-3292

8. References

HEC. Receiving Water Quality Model, Hydrologic Engineering Center, U.S. Army Corps of Engineers, Davis, CA. 95616, 1979.

Abbott, Jess and Willey, R. G. Pennypack Creek Water Quality Study, Hydrologic Engineering Center, U.S. Army Corps of Engineers, Davis, CA. 95616, 1979.

RIVER BASIN MODEL (RIBAM)

1. Model Overview: RIBAM is a modification of the DOSAG water quality prepared by the Texas Water Development Board. The DOSAG model has been expanded to model 17 stream water quality parameters, sulfates, manganese, iron, total nitrogen, dissolved solids, lead, chlorides, phosphorus, ammonia, nitrite, nitrate, cyanide, phenols, BOD, chlorpohyll A, dissolved oxygen, and coliforms. The user supplies streamflow, waste discharge flows and concentrations, and stream physical characteristics. The model calculates the water quality profile for each water quality management alternative.

2. Functional Capabilities: RIBAM is a steady state, one dimensional stream model. For modeling, the river system is sub-divided into segments with uniform physical and hydrologic characteristics. Advection is considered the dominant transport mechanism. Tributaries and waste water discharges are added at segment boundaries. Stream concentrations are computed at the head and end of each segment.

3. Basic Assumptions: RIBAM assumes stream concentrations are either conservative within a segment or behave according to first order reaction kinectics. Point source discharges are assumed to mix completely and are instantaneously minimal. Within each segment concentrations are calculated using an exact solution to the differential equation.

4. Input and Output: RIBAM requires the following inputs: Stream physical characteristics (width, depth and velocity for each segment), upstream conditions (flow and concentrations), effluent flows and concentrations, stream reaction rates for each segment and segment temperatures.

RIBAM provides a copy of all input data and a table summarizing computed stream concentrations for each constituent modeled. Stream concentrations are reported for upstream and downstream ends of each segment for all constituents except dissolved oxygen for which maximum and minimum concentrations and their location are reported in addition to the above.

5. System Resource Requirements: RIBAM may be run on a mainframe similar to the IBM 360 or Univac 1110 series. Core memory requirements are less than 100K bytes and the model is coded in FORTRAN IV. An engineering background is useful in the model's application.

6. Applications: RIBAM was used to determine effluent limitations for municipal and industrial dischargers on the Mahoning River (eastern Ohio). In this study the program option to assess the sensitivity of computed concentrations to various inputs was used in addition to the subroutine which determines dissolved oxygen reaeration at channel dams.

7. Technical Contact:

Donald Schregardus
U.S. Environmental Protection Agency
Region 5, Eastern District Office
25089 Center Ridge Road
Westlake, OH 44145
COM 216/835-5200

8. References:

Raytheon Co., Oceanographic and Environmental Services, *Documentation Report Beaver River Basin Model Project*, March 1973, Contract No. 68-01-0746.

Raytheon Co., Oceanographic and Environmental Services, *Expanded Development of BEBAM-A Mathematical Model of Water Quality for the Beaver River Basin*, May 1974, Contract No. 68-01-1836.

Amendola, G.A., Schregardus, D.R., Harris, W.H., Moloney, M.E., *Mahoning River Waste Load Allocation Study*, September 1977.

RIVER TEMPERATURE SIMULATION MODEL (TEMPSTAT)

1. Model Overview: The computer program TEMPSTAT is a river temperature simulation model developed for assessing numerous thermal loading alternatives for the Mahoning River (eastern border of Ohio, flows through Warren and Youngstown). The Edinger and Geyer temperature decay equations were used for the program with statistically varying inputs to compute the statistical distribution of temperatures at designated points along the river.

2. Functional Capabilities: The model uses a one dimensional steady state temperature calculation procedure developed by Edinger and Geyer. Thermal loadings are input as a mean and standard deviation. TEMPSTAT uses a normal distribution random number generator to determine specific inputs for each calculation. Numerous repetitive stream calculations are made to determine the distribution of temperature in the river.

3. Basic Assumptions: The model assumes that the temperature of heated water discharged to the river decays exponentially to an equilibrium temperature. Complete mixing of the effluent into the receiving stream is assumed as well as a non-stratified uniform temperature distribution at each point in the river. Input loadings, equilibrium temperatures, heat exchange coefficients and stream flows are assumed to be independent variables.

4. Input and Output: TEMPSTAT requires the mean and standard deviation of thermal effluent loadings, flow duration data, stream surface area and the mean and standard deviation of the equilibrium temperature (E), and heat exchange coefficient (K). E and K may be calculated by a separate program requiring hourly meteorological data (air temperature, wind speed, relative humidity and cloud cover).

TEMPSTAT outputs the statistical distribution of stream temperatures at selected points in the river. Outputs include maximum, minimum, mean and standard deviations of the calculated temperatures. Also reported are the temperatures exceeded 1, 5, 10 and 20 percent of the time.

5. System Resource Requirements: This model may be run on a Univac 1110 mainframe with core requirements of less than 100K bytes. It is coded in FORTRAN IV. A programming and an engineering background is useful in this model's application.

6. Applications: TEMPSTAT was used to evaluate thermal loading alternatives on the Mahoning River. With some modification it was also used to compute temperatures in the low Black River (tributary of Lake Erie, West of Cleveland). Equilibrium temperatures and heat exchange coefficients were determined for both rivers using a model developed by the U.S. Army Corps of Engineers and modified to fit program requirements.

7. Technical Contact:

Donald Schregardus
U.S. Environmental Protection Agency
Region 5, Surveillance & Analysis Division
Eastern District Office
25089 Center Ridge Road
Westlake, OH 44145
COM 216/835-5200

8. References:

U.S. Environmental Protection Agency, Eastern District Office, Mahoning River Waste Load Allocation Study, September 1977.

U.S. Environmental Protection Agency, Eastern District Office, Black River Waste Load Allocation Report, September 1980.

User's Manual not presently available.

SIMPLIFIED ESTUARY MODEL (SEM)

1. Model Overview: The Simplifed Estuary Model (SEM) is a one-dimensional, steady state water quality model for the evaluation of uncoupled chemical reactions and BOD-DO deficits in tidal streams and rivers, and non-stratified estuaries. Constituents that can be modeled include BOD, DO, unspecified conservatives, and uncoupled non-conservatives with first order decay (i.e. some nutrients). SEM was developed by Hydroscience, Inc. for the EPA as a "first cut" water quality planning tool to achieve estimates of ambient DO concentrations in estuaries downstream from point source residual inputs. The model requires no computer equipment except for a hand calculator which is used to compute logs and exponentials.

2. Functional Capabilities: SEM is a far-field, one-dimensional (horizontal plane) model that considers only longitudinal variations and handles only point source residual inputs. The model can be applied to tidal streams and rivers, and to non-stratified estuaries. Physical processes that can be represented include advection, longitudinal dispersion, dilution, reaeration, and temperature effects. The model can simulate uncoupled chemical reactions and coupled BOD-DO deficit reactions, and it can represent the following constituents: BOD, DO, unspecified conservatives, and uncoupled non-conservatives with first order decay. No biochemical processes are represented directly, although the modeling of first order decay for coliform bacteria is possible. The simplified nature of SEM restricts its usage when complicated prototype systems or complex water quality problems are involved.

SEM has a moderate estimated sensitivity to residual inputs, stream flow and velocity, and decay coefficients.

3. Basic Assumptions: The model considers only longitudinal variations and handles only point source residual inputs. It assumes a constant velocity for each reach, and assumes first-order decay rates for quality constituents.

4. Input and Output: The following input data is required for initial setup/calibration of the model:

1) Net river flow exclusive of tidal effects
2) Flow velocities
3) Average depths
4) Distance from point source discharges
5) Dispersion coefficients
6) Cross-sectional area
7) Constituent concentration, temperature and background DO for all stream inflows
8) Loading rate for ultimate oxygen demand
9) Deoxygenation coefficients
11) Reaeration coefficients
12) Salinities at the seaward boundary

Constituent concentrations throughout the modeled area are needed for verification of the model.

Output from the model (through hand calculation) includes constituent concentrations, maximum DO deficit, and minimum DO concentrations.

5. System Resource Requirements: SEM is uncoded and requires no computer equipment except for a hand calculator which is used to compute logs and exponentials. Data preparation and model setup (including model familiarization) requires 1-2 man-weeks, and the actual computation time may take from several man-hours to several man-days depending on the complexity of the application and the mathematical skill of the personnel involved. A background in engineering with a mathematical orientation would be useful. No programming experience is necessary.

6. Applications: SEM has been used for various applications.

7. Technical Contact

Robert B. Ambrose
U.S. Environmental Protection Agency
Environmental Research Laboratory
College Station Road
Athens, Georgia 30605
FTS 250-3546 COM 404/546-3546

8. References

Hydroscience, Inc. "Simplified Mathematical Modeling of Water Quality." Report to Office of Water Programs, U.S. Environmental Protection Agency, Washington D.C. (U.S. Government Printing Office No. 1971-44-367/392), 1971.

Hydroscience, Inc. "Addendum to Simplified Mathematical Modeling of Water Quality." Report to Office of Water Programs, U.S. Environmental Protection Agency, Washington, D.C. (U.S. Government Printing Office No. 1972-484-486/291), 1972.

SIMPLIFIED STREAM MODEL (SSM)

1. Model Overview: The Simplified Stream Model is a one-dimensional, steady state water quality model for the evaluation of conservatives, singular non-conservatives with first order decay, and coupled BOD-DO deficits in streams, rivers, and shallow non-stratified lakes. It was developed by Hydroscience, Inc. for the EPA as a "first cut" planning tool to achieve estimates of ambient DO downstream from point sources. SSM requires no computer equipment except for an electric hand calculator which is used to compute logs and exponentials.

2. Functional Capabilities: SSM is capable of simulating the physical processes of dilution, advection, reaeration, and temperature effects in streams, rivers, and shallow non-stratified lakes. Uncoupled chemical reactions can be represented, as well as coupled BOD-DO deficit reactions. Constituents that can be represented by the model include BOD, DO, unspecified conservatives, and un-coupled non-conservatives with first order decay. The model handles only point source residual inputs, and its simplified nature restricts its usage when complicated prototype systems or complex water quality problems are involved. No biochemical processes are represented directly, although first order decay for coliform bacteria may be possible.

SSM has a high estimated sensitivity to residual loading rates and stream velocities, and a moderate estimated sensitivity to decay coefficients and total streamflow.

3. Basic Assumptions: The model considers only longitudinal variations and handles only point source residual inputs. It assumes a constant stream velocity for each reach, and assumes first order decay rates for quality constituents.

4. Input and Output: For intial set-up/calibration needs, the following input data is required:

1) Net river flow
2) Flow velocity

3) Depth
4) Distance from point source discharges
5) Constituent concentration, temperature, and background DO deficit for all stream inflows
6) Loading rate for ultimate oxygen demand
7) Deoxygenation coefficients

Constituent concentrations throughout the modeled area are required for model verification.

Output from the model (through hand calculation) includes constituent concentrations and DO deficits.

5. System Resource Requirements: The model is uncoded and requires no computer equipment except for an electronic hand calculator which is used to compute logs and exponentials. Data preparation and model set-up may require 1-2 man-weeks, and actual computation time may take from several man-hours to several man-days, depending on the complexity of the application and the mathematical skill of the personnel involved. A background in engineering with a mathematical orientation is useful. No programming experience is necessary.

6. Applications: SSM can be applied to rivers, streams. and shallow, non-stratified lakes for the evaluation of conservatives, non-conservatives with first-order decay, and coupled BOD-DO deficits.

7. Technical Contact

Robert B. Ambrose
U.S. Environmental Protection Agency
Environmental Research Laboratory
College Station Road
Athens. Georgia 30605
FTS 250-3546 COM 404/546-3546

8. References

Hydroscience, Inc. "Simplified Mathematical Modeling of Water Quality." Report to Office of Water Programs, U.S. Environmental Protection Agency, Washington, D.C. (U.S. Government Printing Office No. 1971-444-367/392), 1971.

Hydroscience, Inc. "Addendum to Simplified Mathematical Modeling of Water Quality." Report to Office of Water Programs, U.S. Environmental Protection Agency, Washington, D.C. (U.S. Government Printing Office No. 1972-484-486/291), 1972.

STREAM 7B

1. Model Overview: STREAM 7B is a one-dimensional steady - state model, characterized by first-order or coupled first order reaction kinetics. It is primarily intended for use in the analysis of biochemical oxygen demand (BOD) and dissolved oxygen (DO), although it may be applied for any other parameter assumed to follow first-order reaction kinetics.

2. Functional Capabilities: The purpose of this model is to calculate NBOD, CBOD, DO and fecal coliforms as well as an optional constituent at various points within a river system. Average algal photosynthesis and respiration can be modeled. Model can produce plots if desired.

3. Basic Assumptions: The basic assumptions are: constant stream velocity, steady state, first order decay, and reaeration by COVAR`s method.

4. Input and Output: The inputs for this model are: river NBOD oxidation rates, bottom sludge deoxygenation rates, dam reaeration rates, rapids reaeration rate, stream reaeration rates, NBOD settling rate, fecal coliform decay rate, optional constituent decay rate, time of travels, reach lengths, flows, distributed inflow, temperatures, waste discharges, algal production, respiration rates, and mean reach depths.

The outputs for this model are: concentrations of NBOD, CBOD, DO, fecal coliform and an optional constituent at various points within a river system. It also provides plots of algal photosynthesis and respiration over time.

5. System Resource Requirements: STREAM 7B is coded in FORTRAN IV and can be run on the IBM 370/168 or any equivalent mainframe computer. It requires less than 300K bytes of core storage for execution. It uses any 132 position line printer for output. A background in programming and engineering is helpful.

6. Applications: STREAM 7B is used in waste load allocations.

7. Technical Contact

Douglas A. Little
U.S. Environmental Protection Agency
JFK Federal Building
Boston, MA 02203
COM 617/223-5885 FTS 223-5885

8. References

Resource Analysis, Inc. STREAM 7A User`s Manual, March 1978.

Resource Analysis Addendum to STREAM 7A User`s Manual - STREAM 7B, June 1980.

STREAM NETWORK SIMULATION PROGRAM (SNSIM)

1. Model Overview: SNSIM is a computer program for the steady-state water quality simulation of a stream network. Its basis is an expanded form of the Streeter-Phelps equation, and it is designed to evaluate and/or predict the DO and the carbonaceous and nitrogenous BOD profiles in a river or stream where the effects of dispersion can be assumed to be insignificant. This environmental model is ideal for the evaluation of various water treatment schemes, as its basic control variable is waste input.

2. Functional Capabilities: SNSIM can be used to formulate a steady-state, one-dimensional simulation model of a stream network. The stream network consists of a river and its tributaries which are segmented into sections of constant hydrologic, physical, chemical, and biological parameters. Loads may be applied pointwise at the ends of the section or as distributed sources along its length. BOD loads include carbonaceous and nitrogenous point loads and distributed loads, while DO deficit loads include the distributed loads of benthal demand and photosynthetic demand. Point sources of both BOD and DO deficit from minor tributaries can be input at the ends of a section, and background loads of BOD and DO deficit can be introduced at the system's upstream ends. SNSIM is limited to combining a maximum of 4 tributaries at one confluence, and the number of reaches that may be stored at one time is 10, but these limits may be expanded by changing the dimension statements for these variables.

3. Basic Assumptions: This model typifies the sanitary engineering approach in that its emphasis is on relating man's waste inputs to the aquatic environment with the express purpose of managing the inputs and thus the water quality. An expanded form of the Streeter-Phelps equation is the basis of the SNSIM computer program, and the model is designed to evaluate and/or predict the dissolved oxygen, and the carbonaceous and nitro-

genous BOD profiles in a river or stream where the effects of dispersion can be assumed to be insignificant.

4. Input and Output: SNSIM requires a large input data base which must be in card-image form. For each reach the following information should be provided: Instream flow, instream carbonaceous demand, instream nitrogenous demand, instream DO deficit, increment size for a section output, an integer representing the reach number of the starting mile-point, the number of sections in the reach, the number of tributaries or reaches to be combined, and the indicator which designates if the reaeration rate is to be input or computed. A control variable which indicates if the stream depth, flow, and velocity are to be computed by exponential correlation equations may also be used.

The section length, stream depth, stream velocity, waste or effluent flow at the head of the section, effluent COD, effluent NOD, effluent DO deficit, tributary flow at the head of the section, and the ratio of ultimate to 5-day BOD are needed. In addition, the tributary COD, tributary NOD, the tributary DO deficit, water temperature, carbonaceous BOD deoxygenation rate, carbonaceous BOD decay rate, nitrogenous BOD decay rate, reaeration rate, algal oxygen rate, benthic oxygen demand, the carbonaceous and nitrogenous bank loads, and the altitude above sea level are required.

Reports produced by the SNSIM program include the input parameters for each reach, as well as converted reaction rates, section numbers, section names, distance downstream, CBOD, NBOD, DO, flow, deficit components, and the total deficit for each reach.

5. System Resource Requirements: The SNSIM/1 is written in FORTRAN IV for use on the IBM 370/155 in a 16K area of core storage. It may also be modified for compatibility with the IBM 1130 (SNSIM/2). A background in programming or environmental engineering with experience in water quality modeling are helpful for the model.

6. Applications: SNSIM has been used for various applications within the Environmental Protection Agency.

7. Technical Contacts

George A. Nossa and Laura Livingston
U,S. Environmental Protection Agency
Information Systems Branch 2PM-IS
26 Federal Plaza
New York, New York 10278
FTS 264-9850 COM 212/264-9850

Steven C. Chapra
NOAA Great Lakes Environmental Research Laboratory
2300 Washtenaw Avenue
Ann Arbor, Michigan 48104
FTS 378-2250 COM 313/668-2250

8. References

Braster, R.E., Chapra, S.C., and Nossa, G.A., Documentation for SNSIM1/2, A Computer Program for the Steady-State Water Quality Simulation of a Stream Network, U.S. Environmental Protection Agency, Region II, 26 Federal Plaza, New York, New York, March 1978.

STREAM QUALITY MODEL (QUAL-II)

1. Model Overview: QUAL-II is designed to simulate the dispersion and advection of conservative and reacting constituents in branching stream system and rivers. Constituents modeled include conservative minerals, temperature, BOD, chlorophyll a, phosphorus, ammonia, nitrate, nitrite, DO, coliform bacteria, radioactive material, and an arbitrary nonconservative material. It also considers nutrient cycles and algal growth. The program simulates the dynamic behavior of these constituents by numerical integration of the one-dimensional form of the advection-dispersion transport equation. A steady-state solution of the equations is also available in the program. Any branching stream system can be simulated.

2. Functional Capabilities: QUAL-II represents the stream simulated through the use of reaches. A reach is defined as a stretch of the stream with uniform hydraulic characteristics. Each reach is divided into computational elements. A maximum of 75 reaches, each with up to 20 computational elements with no more than 500 in the system, can be accommodated in the standard version of the program. In addition, there can be a total of 15 headwater elements, 15 junction elements, and 90 input and withdrawal elements. All input is in relation to each reach, and the hydraulics equations are solved by incorporating advection and dispersion through a finite difference implicit solution technique. The results on the quality constituents are obtained by numerical integration of the one dimensional form of the advection-dispersion mass transport equation for each constituent. The model proceeds to solve the relevant equations of each constituent until a steady state equilibrium is achieved. QUAL-II is written in a modular fashion so as to facilitate the incorporation of additional processes.

3. Basic Assumptions: QUAL-II assumes first order kinetics and it utilizes a simplified nutrient-algae cycle with Monod kinetics. Only constant inflows and point source discharges are considered, and each computational element is considered completely mixed. The model does not consider variations in depth or within stream cross-section.

4. Input and Output: QUAL-II requires an input data base in card-image form. Aside from the printed report, no additional requirements are imposed. The data required are varied and includes evaporation coefficients, oxygen uptake per unit of nitrogen and unit of algae, algal growth rates, nitrogen and phosphorus half saturation constants, and reaction rate constants. Further input required is the identification of the computational elements and their hydraulic characteristics, and the initial conditions of the system.

The printed output includes a complete history of every quality parameter and temperature at each computational element. The hydraulic information provided includes the flow, velocity, and depth of each reach, as well as at the head of the system. Water quality information provided includes the concentration of each quality component, the temperature, and the reaction rates at each computational element in the system.

5. System Resource Requirements: The model is written in FORTRAN IV (G) and may be installed on any digital computer with at least 45,000 words of core storage and a FORTRAN IV compiler. A version of the program with reduced capabilities is available that will execute on EPA s PDP 11/70 scientific computers and may be used on other minicomputers. It requires

4-10 weeks of effort for the data preparation and report interpretation. An operator with computer programming and environmental engineering experience is useful.

6. Applications: QUAL-II can be used to simulate the dispersionary and flow characteristics of conservative and non-conservative constituents in branching stream systems and rivers. It is a modification of the QUAL-I Model that was developed by the Texas Water Development Board. The version currently (May 82) distributed by EPA was modified for the Southeast Michigan Council of Goverments and has been extensively reviewed and tested. Training in the use of the model is available through the center for Water Quality Modeling. It is widely used in Wasteland Allocation studies.

7. Technical Contact

Tom Barnwell
U.S. Environmental Protection Agency
Center for Water Quality Modeling
Athens, GA. 30613
COM 404/546-3585 FTS 250-3585

8. Reference

Brown, L.C. "A Review of the Mathematical Water Quality Model QUAL-II and Guidance for Its Use." Technical Bulletin 338, National Council of the Paper Industry for Air and Stream Improvement, Inc., 260 Madison Ave., New York, Oct. 1980.

Roesner, L.A., Giguere, P.R., and Evenson, D.E. Computer Program Documentation for the Stream Quality Model QUAL-II, EPA-600/9-81-014, USEPA, Athens, GA, Feb. 1981.

Roesner, L.A., Giguere, P.R., and Evenson, D.E. "Users Manual for the Stream Water Quality Model QUAL-II," EPA-600/9-81-015, USEPA, Athens, GA, Feb. 1981.

Whittemore, R.C. and Hovis, J. "A Study of the Selection, Calibration and Verification of Mathematical Water Quality Models." Technical Bulletin 367, National Council of the Paper Industry for Air and Stream Improvement, Inc., 260 Madison Ave., New York, March 1982.

TIDAL TEMPERATURE MODEL (TTM)

1. Model Overview: The Tidal Temperature Model (TTM) is a derivative of the Dynamic Estuary Model (DEM) that can simulate the heat budget and dispersional characteristics of streams, well-mixed shallow impoundments, estuaries, and coastal waters. The model can accomodate constituents which may be conservative or non-conservative, have coupled or non-coupled reactions, and which undergo first order decay. The TTM was developed by the EPA Pacific Northwest Laboratory and has been applied to the Columbia River below the Bonneville Dam.

2. Functional Capabilities: The TTM represents the one dimensional tidal and net river flow, transport processes of advection and diffusion, the heat budget and the dilution of up to four constituents within an estuary, stream, well-mixed shallow impoundment, or coastal waters. Coupled BOD-DO reactions may be modeled, as well as up to four constituents which may be conservative or non-conservative, have coupled or non-coupled reactions, and undergo first order decay. The model can simulate systems with up to 300 channels and as many as 300 junctions. The TTM primarily links hydrodynamic and temperature/heat budget components, but additional water quality constituents may be possible. A standard heat budget approach and a thermal equilibrium approach are used to figure temperatures.

3. Basic Assumptions: The TTM assumes that all inflows or withdrawals are constant, and it utilizes a simplified form of evaporation. One dimensional channels are used to represent two dimensional flows and transports. The model neglects wind stress and disregards lateral and vertical variation in channel cross-sectional area with tidal elevation change. It handles constant residual input rates which can be put in variable form, and it cannot simulate tidal flats that go dry.

4. Input and Output: The Tidal Temperature Model allows for a large input data base, written in card-image form. Parameters

which can be specified include headwater flows, tributary flows, groundwater flows, water withdrawals, seaward tides, channel depths and widths, bottom roughness, constituents in freshwater inflows and at seaward boundaries, constituent concentrations throughout the modeled area, the quality and quantity of point-source residuals discharges, net solar radiation, and wet and dry bulb temperatures.

Output formats include tabular printouts and velocities written by the hydrodynamic module. Output information provided by the model includes summarized data (maximum and minimum values) for tidal cycles, flows, velocities, water elevation, constituent concentrations at each junction, channel velocities, junction depths, and constituents at user specified periods.

5. System Resource Requirements: The TTM is written in FORTRAN IV and can be run on any digital computer with at least 50,000 words of main storage and a FORTRAN IV compiler. Operator skills required include experience in hydrodynamic and water quality modeling and programming. The model requires 5-20 manweeks for data preparation and several manhours for output interpretation.

6. Applications: The Tidal Temperature Model has been used by the EPA Pacific Northwest Water Laboratory and has been applied to the Columbia River below the Bonneville Dam. The model has also been used by the EPA in Massachusetts, South Carolina, Florida, Oregon, and Washington.

7. Technical Contact

Richard J. Callaway
U.S. Environmental Protection Agency
Corvallis Environmental Research Laboratory
200 S.W. 35th Street
Corvallis, Oregon 97330
FTS 420-4703 COM 503/757-4703

8. References

Callaway, R.J. and Byram, K.V . "Mathematical Model of the Columbia River from the Pacific Ocean to Bonneville Dam, Part II: Input-Output and Initial Verification Procedures." Report by U.S. EPA Pacific Northwest Water Laboratory, Corvallis, Oregon, 1971.

Callaway, R.J., Byram, K.V., and Ditsworth, G.R. "Mathematical Model of the Columbia River from the Pacific Ocean to Bonneville Dam, Part I. Theory, Program·Notes and Programs." Report by FWQA Pacific Northest Water Laboratory, Corvallis, Oregon, 1969.

TIME-DEPENDENT, THREE-DIMENSIONAL TRANSPORT MODEL

1. Model Overview: The time-dependent, three-dimensional transport model was developed to calculate the hydrodynamic transport of conservative and non-conservative substances in various water bodies. The model calculates the time-dependent concentration of the desired substance. Input to this model for velocities are results from the separately described hydrodynamic model. Various user specified options permit application to conservative substances such as chloride and non-conservative substances such as suspended solids.

2. Functional Capabilities: The model is fully time-dependent and three-dimensional. The spatial resolution is up to the discretion of the modeler but is usually the same as used in the hydrodynamic model. The time step restrictions are dependent on the particular application. The vertical diffusion term in the equation is calculated implicitly in time so there is no time step stability restriction for this term. The other terms in the equations are treated explicitly. Various combinations of boundary conditions can be used. For suspended solids calculations, flux at the water-sediment interface is parameterized by 2 coefficients determined by laboratory experiments. Conservation-perserving finite difference techniques are used.

3. Basic Assumptions: The equations are derived from the time-dependent, three-dimensional equation for conservation of material. The main assumption is that eddy coefficients are used to account for turbulent diffusion effects. The program for the model is modular in form so this condition can be changed to incorporate various turbulence modeling schemes.

4. Input and Output: Input to the model includes: complete specification of geometry and grid layout (which can be obtained from hydrodynamic model), topography, and forcing. The latter includes velocities (from hydrodynamic model), inputs/outputs, and other things such as wind depending on what is being modeled. The initial conditions can be user specified or from results of previous calculation.

The basic output of the program is a printed record of concentrations, as desired. If results are stored (disk or tape), separate programs are available to produce graphic output on either Tektronix or Calcomp equipment. The plots available include time series and horizontal and vertical sections.

5. System Resource Requirements: This model is coded in FORTRAN and can be run on an IBM 370/4300, Univac 1100, VAX 11/780 and Cray mainframe. It requires between 50k and 1.5 m words core storage. It uses a high speed line printer for output. It requires a card reader/punch if disk input is not used. A background in scientific computer programming and hydrodynamic modeling is helpful.

6. Applications: The model has been applied to the following: Lake Erie, entire basins of Lake Erie, Saginaw Bay, Sea of Azov, Lake Baikal and Waukegan Harbor. Organization that have used the model include various federal agencies and universities in this country and in Europe.

7. Technical Contact

Dr. John F. Paul
U.S. Environmental Protection Agency
Environmental Research Laboratory
South Ferry Road
Narragansett, RI 02882
COM 401/789-1071 FTS 838-4843

8. References

Lick, W.J., Paul, J., and Sheng, Y.P., The Dispersion of Contaminants in the Near-Shore Region. In: Modeling Biochemical Processes in Aquatic Ecosystems (R.P. Canale, ed.). Ann Arbor Science Publishers, Inc. pp. 93-112, 1976.

Paul, J.F., and Patterson, R.L., Hydrodynamic Simulation of Movement of Larval Fishes in Western Lake Erie and their Vulnerability to Power Plant Entrainment. Proc. of the 1977 Winter Simulation Conf. (H.J. Highland, R.G. Sargent and J.W. Schmidt, ed.), WSC Executive Committee, pp. 305-316, 1977.

Paul, J.F., Richardson, W.L., Gorstko, A.B., and Matveyev, A.A., Results of a Joint USA/USSR Hydrodynamic and Transport Modeling Project. EPA-600/3-79-015, 1979.

TIME-DEPENDENT, THREE-DIMENSIONAL, VARIABLE-DENSITY HYDRODYNAMIC MODEL

1. Model Overview: The time-dependent, three-dimensional, variable density hydrodynamic model was developed to describe the motion in thermal discharges in harbors, bays, lake basins, entire lakes, estuaries, etc. The model calculates velocities and temperature (salinity, also, if required) as a coupled set of time-dependent, non-linear partial differential equations. The results of the model can be used as input to a transport model (described separately). The model has various versions (user specified) such that the calculations can be performed with the water surface treated rigid-lid or as a free-surface and with the bottom boundary condition specified either as no-slip or slip.

2. Functional Capabilities: The model is fully time-dependent and three-dimensional. The spatial resolution is up to the discretion of the modeler and the time step restrictions are dependent on the individual application. The Coriolis, pressure, and vertical diffusion terms in the equations are calculated implicitly in time, so no time step stability restiction applies to them. The other terms are calculated explicitly. The momentum and energy (and salinity) equations are coupled. Various combinations of boundary conditions can be used at the discretion of the modeler.
Conservation-preserving finite difference techniques are used.

3. Basic Assumptions: The equations are derived from the time-dependent, three-dimensional equations for conservation of mass, momentum, energy, and salinity. The principal assumptions are: 1. hydrostatic pressure variations 2. rigid-lid or linearized free-surface approximation and 3. eddy

coefficients to account for turbulent diffusion effects. The program for the model is modular in form so the last condition can be modified to account for various turbulence modeling schemes. The solution procedure is a modification of the simplified marker and cell technique.

4. Input and Output: Input to the model includes: complete specification of geometry and grid layout, topography, and forcing functions. The latter includes wind (constant or spatial and temporal varying), inflows/outflows, and heat specification at water surface. The initial conditions can be quiescent conditions, some user specified form, or results from previous calculation.

The basic outputs of the program are a printed record of velocities, temperature, salinity and pressure, as desired. If results are stored (disk or tape), separate programs are available to produce grahic output on either Tektronix or Calcomp equipment. The plots available include time series of variables, and horizontal and vertical section plots of the variables.

5. System Resource Requirements: This model is coded in FORTRAN and can be run on an IBM 370/4300, Univac 1100, VAX 11/780, or Cray mainframe. It requires between 50k and 1.5 M words core storage. It uses a high speed line printer for output. It requires a card reader/punch if disk input is not used. A background in scientific computer programming and hydrodynamic modeling is helpful.

6. Applications: The model has been applied to the following: Lake Huron; Lake Erie; separate basins of Lake Erie; the area of Lake Erie for proposed jetport; Cleveland harbor; vicinity of Monroe, Michigan for proposed dredged spoil sites; Saginaw Bay; numerous thermal discharges in the Great Lakes and the Baltic Sea; Sea of Azov; Lake Baikal; and Waukegan Harbor.

Organizations that have used the model or results of the model include Corps of Engineers, Swedish Meteorological and Hydrological Institute, Argonne National Laboratory, Rudjer Boskovic Institue (Yugoslavia), Hydrometeorological Institute (USSR), Ohio State University, University of Arizona, NASA, NOAA, University of California, and U.S. EPA.

The output of the model can be used directly in a separate transport model.

7. Technical Contact

Dr. John F. Paul
U.S. Environmental Protection Agency
Environmental Research Laboratory - Duluth
South Ferry Road
Narragansett, RI 02882
COM 401/789-1071 FTS 838-4843

8. References

Lick, W.J., Paul J., and Sheng, Y.P. The disperison of contaminants in the near-shore region. In: Modeling Biochemical Processes in Aquatic Ecosystems (R.P. Canale, ed.) Ann Arbor Science Publishers, Inc. pp.93-112, 1976.

Paul, J.F. Modeling the Hydrodynamic Effects of Large Man-Made Modifications to Lakes. Proc. of the EPA Conf. on Environmental Modeling and Simulaton (W.R. Ott, ed.). EPA-600/9-76-016, pp. 171-175, 1976.

Paul, J.F. and Lick, W.J. A Numerical Model For a Three-Dimensional, Variable-Density Jet. Report No. FTAS/TR73-92, School of Engineering, C.W.R.U., Cleveland, Ohio, 1973.

Paul, J.F. and Lick W.J., A Numerical Model For a Three-Dimensional, Variable-Density Jet. Proc. 16th Conf. Great Lakes Res., IAGLR, pp. 818-830, 1973.

Paul, J.F. and Lick, W.J., A Numerical Model for Thermal Plumes and River Discharges. Proc. 17th Conf. Great Lakes Res., IAGLR, pp. 445-455, 1974.

Paul, J.F. and Lick, W.J., Report to Argonne National Laboratory of the Application of the Paul-Lick Model to Point Bench Unit 1 Outfall. Appears in appendix of Surface Thermal Plumes: Evaluation of Mathematical Medals for the Near and Complete Field (W.E. Dunn, A.J. Policastro and R.A. Paddock), ANL/WR-75-3, pp. 484-511, 1975.

Paul, J.F. and Lick, W.J., Application of Three Dimensional Hydrodynamic Model to Study Effects of Proposed Jetport Island on Thermocline Structure in Lake Erie. Report 17-6 of Lake Erie International Jetport Model Feasibility Investigation. U.S. Army Engineer Waterways Experimental Stations Contract Report H-75-1, 1976.

Paul, J.F. and Lick, W.J., An Efficient, Implicit Method for Calculating Time-Dependent, Free-Surface, Hydrodynamic Flows. Presented at the 22nd Conference on Great Lakes Research, Rochester, New York, 1979.

Paul, J.F. and Lick W.J., Numerical Model for Three Dimensional, Variable-Density Rigid-Lid Hydrodynamic Flows: Volume 1. Details of the numerical model. In preparaton, 1980.

Paul, J.F., Richardson, W.L., Gorstko, A.B. and Matveyou, A.A., Results of a Joint USA/USSR Hydrodynamic and Transport Modeling Project EPA-600/3-79-015, 1979.

Vasseur, B., Funkquist, L., and Paul, J.F., Verification of a Numerical Model for Thermal Plumes. SMHI Hydrology and Oceanography Report No. 24, 1980.

WATER QUALITY ASSESSMENT METHODOLOGY
FOR TOXIC AND CONVENTIONAL POLLUTANTS (WQAM)

1. Model Overview: The Water Quality Assessment Methodology is a collection of formulas, tables, and graphs which planners can use to perform a preliminary (screening) assessment of surface water quality in large basins. Analyses require little data, and in most cases, can be accomplished with the assistance of a desk top calculator. Desk top calculation procedures are provided for the following subject categories:

Environmental chemistry, including equilibrium and transformation process.

Wasteload estimation, including point and non-point source pollutants.

Stream analyses for toxic organic chemicals, priority pollutants, water temperature, biochemical oxygen demand, dissolved oxygen, total suspended solids, coliform bacteria, plant nutrients, and conservative constituents.

Lake analyses for toxic organic chemicals, priority pollutants, thermal stratification, sediment accumulation, phosphorus budget, eutrophication potential, and hypolimnion DO.

Estuarine analyses for estaurine classification, toxic organic chemicals, priority pollutants, temperature, BOD, DO, turbidity, sediment accumulation, and conservative constituents.

2. Functional Capabilities: This methodology predicts far-field, average steady-state conditions in streams, lakes, and estuaries as a function of long term average maximum and minimum nonpoint source loads and point source loads.

Longitudinal concentration variations are predicted for streams and estuaries. The accuracy is sufficient to bracket expected conditions in a "screening" exercise.

3. Basic Assumptions: The nonpoint source loading section is based on the modified Universal Soil Loss Equation. The stream section is based on steady-state, plug flow solutions to the conservation of mass equation. The lake section is based on empirical stratification relationships and mass balance. The estuary section is based on the modified tidal prism and/or fraction of fresh water formulas.

4. Input and Output: The methodology is designed to operate with minimum data, recognizing that the more data available, the more accurate the analysis. Basic information needed includes: land use, stream lengths and net flows, reservoir depths and volumes, and estuary salinity distributions. Point source loading data is also needed, as well as pollutant properites.

Output from the model includes predicted stream concentrations of BOD, DO, total N, total P, temperature, toxic organic polutants, priority pollutants, and conservative pollutants by reach; total lake nutrient, toxic organic, priority pollutant concentrations, eutrophic status, and hypolimnion DO deficit; and estuary concentrations of BOD, DO, total N, total P, toxic organic, priority and conservative pollutants by reach. Calculations are done by hand calculator and can be arranged to the user's convenience.

5. System Resource Requirements: This model uses a calculator. An engineering background is useful.

6. Applications: The methodology has been applied and tested on the Sandusky River Basin and four Chesapeake Bay sub-basins: the Patuxent, Chester, Ware, and Occoquan. This work was done by the Midwest Research Institute and Tetra Tech on a grant from EPA. The methodology is linked to the Midwest Research Institue loading functions.

The Environmental Protection Agency sponsors training in the use of the methodology from time to time. Further information is available from the Technical Contact.

7. Technical Contact

Thomas O. Barnell, Jr.
U.S. Environmental Protection Agency
EPA Athens Environmental Research Laboratory
Center for Water Quality Modeling
Athens, GA 30613
COM 404/546-3585 FTS 250-3585

8. References

Water Quality Assessment: A Screening Method for Nondesignated 208 Areas, EPA 600/9-77-023, August 1977. Available from NTIS (PB277161/AS for $29).

"Water Quality Assessment Methodology for Toxic and Conventional Pollutants." (in Press), Center for Water Quality Modeling, USEPA, Athens, GA 30613

WATER QUALITY FEEDBACK MODEL (FEDBAK03)

1. Model Overview: FEDBAK03 is used to compute the steady-state distribution of water quality variables undergoing consecutive reactions with feedback and following first order kinetics. The program has been developed in a general form but is specifically applicable to the reactions observed by nitrogenous species and the associated dissolved oxygen uptake in the natural environment. The basis for this model is the theory of conservation of mass. The approach used to solve the equations is a finite difference scheme developed by Thomann, which has been shown to be a very effective tool in the field of water quality management.

2. Functional Capabilities: FEDBAK03 has been developed to help predict water quality parameters which react under first order kinetics and as a system of consecutive reactions, where any parameter can react in a feedback fashion. The problem setting assumes an aquatic environment in which steady-state conditions can be applied. The Thomann solution of solving the general estuarine advection/dispersion equation by replacing the derivatives with finite-difference approximations is the approach followed in FEDBAK03. Optionally, the program can also perform system sensitivity analysis by varying the waste vector and re-multiplying by $[\bar{A}]^{-1}$ and/or changing the reaction rate constants for any reactants and repeating several steps. A second option is the computation of dissolved oxygen deficit and the corresponding dissolved oxygen concentration by selecting the reaction schemes producing the deficit and the associated stochiometric coefficients.

As presently written, the program can accomodate a multi-dimensional system of up to 60 sections and each section can have a maximum of six interfaces. The maximum number of reactants is such that when multiplied by the number of sections, it cannot exceed 120. This present limitation can easily be expanded.

3. Basic Assumptions: The model assumes steady-state conditions in an aquatic environment. It is based on the theory of conservation of mass and utilizes a finite difference scheme for the solution of the general estuarine advection/dispersion equation. Reactants are assumed to undergo consecutive reactions with feedback and first order kinetics.

4. Input and Output: FEDBAK03 requires the input of the physical characteristics of the system to be evaluated; namely, the geometry, temperature, hydrologic characteristics, reaction schemes, and corresponding reaction rates.

5. System Resource Requirements: The computer program has been written for the IBM 370 with a FORTRAN IV (G or H) level compiler. The program occupies 140 K of core to execute and takes 35 CPU seconds to solve a 10 segment, 8 component system. A background in computer programming or environmental engineering with experience in computer modeling is useful.

6. Applications: FEDBAK03 can be used for the calculation of BOD deficit and nitrification.

7. Technical Contacts

George A. Nossa and Laura Livingston
U.S. Environmental Protection Agency
Information Systems Branch
26 Federal Plaza
New York, New York 10278
FTS 264-9850 COM 212/264-9850

8. References

Nossa, G.A., "FEDBAK03 A Computer Program for the Modeling of First Order Consecutive Reactions with Feedback Under a Steady State Multidimensional Natural Aquatic System". Environmental Modeling and Simulation, USEPA Office of Research and Development, Washington, D.C. July 1976.

Nossa, G.A., "FEDBAK03 - Program Documentation and User's Guide" USEPA, Region II, New York, New York, November 1978.

WATER QUALITY FOR RIVER-RESERVOIR SYSTEMS (WQRRS)

1. Model Overview: WQRRS was developed and is supported by the U.S. Army Corps of Engineers' Hydrologic Engineering Center. The WQRRS model (HEC, 1978a) consists of three separate but integrable modules: the reservoir module, the stream hydraulic module, and the stream quality module. The three computer programs may be integrated for a complete river basin water quality analysis through automatic storage of results. An output tape may be generated for input to a separate plotting and statistical program called the Statistical and Graphical Analysis of Stream Water Quality Data (HEC, 1978b).

The system is based on a comprehensive lake ecological simulation program originally developed by Chen and Orlob (1972) and a river simulation model developed by Norton (1972). The original river routines only simulated steady hydraulic conditions so the capability to dynamically route streamflow using either the St. Venant equations, Kinematic Wave, Muskingum, or Modified Pulse method was added. Subsequent updating of the system added the capability to analyze branched and looped stream systems and added additional water quality and biological constituents (King, 1976; Smith, 1978). A separate program for statistical and graphical analyses of stream water quality data is available (HEC, 1978b).

2. Functional Capabilities: The methodology in the reservoir section is applicable to aerobic impoundments that can be represented as one-dimensional systems with horizontal isotherms. The stream hydraulic module includes six hydraulic

computation options capable of handling hydraulic behavior within both the "gradually varied" steady and unsteady flow regimes. The stream quality module simulates transport of quality parameters in aerobic streams.

Physical processes modeled in WQRRS include advection, diffusion, dilution, and the heat budget. Temperature effects on water density and various kinetic parameters are considered. State variables include 18 highly interconnected physical, chemical and biological parameters: BOD, organic detritus, organic sediment, coliform, total carbon, phosphate, ammonia, nitrites, nitrate, DO, pH, total alkalinity, total dissolved solids, carbon dioxide, two algae species, zooplankton, fish, and benthic animals. The river module also includes aquatic insects, benthic algae, suspended solids, and inorganic sediment.

3. Basic Assumptions: WQRRS simulates reservoirs as a one-dimensional vertical plane, and stream segments as a one-dimensional horizontal plane.

4. Input and Output: The initial setup/calibration needs are: flowrate for all lake and stream inflows; lake and stream hydrogeometric data; lake outflow elevations and locations; latitude and longitude of prototype systems; Secchi disc depth for light extinction; concentrations of quality constituents, biological parameters, and temperatures in all lake inflows and river segments throughout the simulation period; initial conditions of quality constituents, biological parameters, and temperatures in each lake layer and river segment; all kinetic parameters, including growth rates, decay rates, respiration rates, settling velocities, mortality rates, and other chemical-ecologic reaction rates; temperature stability coefficients; meteorological data-air temperature (wet and dry bulb); and atmospheric pressure, wind speed, and sky cover.

Verification needs are: the conditions of quality constituents, biological parameters, and temperatures during the simulation period (the vertical profile for lakes, the horizontal profile for river sediments); the constituent concentrations, biological parameters, and temperatures at the lake outflow for specified time periods; and the time history of the lake water surface elevations during simulation.

Output information includes: the time history of quality constituents, temperatures, and biological parameters in each lake layer and river segment; the time history of quality constituents, temperatures, and biological parameters in lake outflows; and all the input values specified. The output format is a tabular printout. Reservoir outflows to river system may be recorded on cards or magnetic tape.

5. System Resource Requirements: The model is coded in FORTRAN IV. Requirements are for 50,000 words storage capacity on Univac 1108. WQRRS can be successfully run on Univac 1108, IBM 360/50, CDC 7600, and Honeywell 600 series.

Pesonnel requirements include computer programming and experience in water quality engineering. Additional experience and expertise in biology and water chemistry are needed to establish proper ecological relationships. Previous experience in detailed water quality models is useful because of the potentially large data base needed for WQRRS.

6. Application: The documentation report costs $14 and can be obtained from the Hydrologic Engineering Center in Davis, California. The complete computer programs can be obtained from HEC for $120. Model setup and data preparation require about 6-18 weeks, depending upon the data base size. Actual computer cost ranges from $30-100 per run, depending upon the

system size and extent of discretization, length of simulation, and number of constituents considered. Output analysis requires several manhours to evaluate each simulation run.

7. Technical Contact

R. G. Willey
Hydrologic Engineering Center
Corps of Engineers
609 Second Street
Davis, California 95616
COM 916/440-3292 FTS 448-3292

8. References

Chen, C. W. and Orlob, G. T. Ecologic Simulation of Aquatic Environments, Office of Water Resources Research, U.S. Dept. of Interior, Washington, D.C, 1972.

King, I. P. Flow Routing for Branched River Systems, prepared for Hydrologic Engineering Center, U.S. Army Corps of Engineers, Davis, CA 95616, 1976.

Norton, W. R. An Assessment of Water Quality in the Lower American River: Past, Present, and Future, County of Sacramento, Dept. of Public Works, Sacramento, CA 95616, 1972.

HEC. Water Quality for River Reservoir Systems, Hydrologic Engineering Center, U.S. Army Corps of Engineers, Davis, CA 95616, 1978.

HEC. Statistical and Graphical Analyses of Stream Water Quality Data, Hydrologic Engineering Center, U.S. Army Corps of Engineers, Davis, CA 95616, 1978.

Smith, D. J. Revised Water Quality for River-Reservoir Systems Model, prepared for Hydrologic Engineering Center, U.S. Army Corps of Engineers, Davis, CA 95616, 1978.

Willey, R. G. and Huff, D. Chattahoochee River Water Quality Analysis, Hydrologic Engineering Center, U.S. Army Corps of Engineers, Davis, CA. 95616, 1978.

Willey, R. G., Abbott, J. and Gee, M. Oconee River Water Quality and Sediment Analysis, Hydrologic Engineering Center, U.S. Army Corps of Engineers, Davis, CA. 95616, 1977.

WATER QUALITY MODEL (EXPLORE-I)

1. Model Overview: EXPLORE-I is a comprehensive mathematical water quality model to be used in river basin planning and water resource studies. This generalized river basin water quality model can predict the hydrodynamics and water quality dynamics for rivers and well mixed estuaries. The EXPLORE-I model is an extended and modified version of the Storm Water Management Model, receiving water component, which was developed for studies of DO/BOD dynamics. The model is capable of simulating a number of hydraulic regimes in either a dynamic or steady state mode, and it has been set up, calibrated, and verified on a portion of the Williamette River Basin, consisting of major tributaries. EXPLORE-I was developed by Battelle-Northwest Laboratories for the EPA.

2. Functional Capabilities: EXPLORE-I can be used to study the effects of various flow conditions, waste discharge and/or treatment schemes on the water quality levels in the river basin. EXPLORE-I is capable of simulating a number of hydraulic regimes in either a dynamic or steady state mode. These are: 1) streams and rivers, 2) shallow lakes, and 3) estuaries or tidally influenced rivers. In addition, the behavior of the following water quality parameters can be studied:

1) Carbonaceous Biochemical Demand (BOD)
2) Nitrogenous BOD
3) Benthic BOD
4) Total Organic Carbon (TOC)
5) Refractory Organic Carbon
6) Sedimentary Phosphorous
7) Soluble Phosphorous
8) Organic Phosphorous
9) Ammonia Nitrogen

10) Nitrite Nitrogen
11) Nitrate Nitrogen
12) Organic Nitrogen
13) Toxic Compounds
14) Phytoplankton
15) Zooplankton
16) Dissolved Oxygen

EXPLORE-I is composed of a river basin program which is capable of modeling one-dimensional open channel flow in streams and rivers, and two-dimensional flow in shallow lakes and estuaries. The program consists of a hydraulic code which calculates the required water velocities, depths, and flows, and a quality code which evaluates the quality parameter reactions and routes the constituents through the system. The model is capable of simulating diurnal or long-term periods, and it can handle constant and/or time-varying point or diffuse sources.

3. Basic Assumptions: The overall model formulation is partitioned into two basic modules which can be operated sequentially: a hydrodynamics module and a mass transport and water quality submodels module. The hydrodynamics module is formulated on conservation of mass and momentum principles. The mass transport and water quality submodels module is formulated from the expressions for specie continuity, i.e., mass balance of a particular constituent or specie. For any biotic or abiotic substance the general mass transfer expression is the sum of the individual forms of mass transfers. Diffusion is assumed to be negligible, and mass transfer is partitioned into simple transport and water quality kinetics.

4. Input and Output: Junction and channel data are required for the hydrodynamics module. Junction input data include:

1) The average water surface elevation for the junction point
2) The water surface area associated with the junction point
3) Any significant inflows to the junction point from small streams, tributaries, or other sources
4) Any significant outflows from the junction point
5) The average elevation of the bottom of the river or estuary for the junction point
6) The cartesian coordinates of the junction point (necessary only if the effect of wind stress on channel flow is being calculated)

Required input channel data include:

1) Channel length
2) Channel width
3) Average elevation of the channel bottom
4) Manning coefficient for the channel
5) Initial velocity in the channel

Input for the water quality program include: upstream node specification, reach boundaries, source node specification, BOD constants, benthic BOD constants, TOC constants, toxic constants, DO production by phytoplankton, DO production by benthic plants, reaeration constants, phosphorous constants, nitrogen constants, algae constants, number of constant sources, constant source values, time-varying source values, reach temperatures, constant upstream node concentrations, and time-varying upstream node concentrations.

Output produced by the model includes an echo of the input data and BOD and loading rates for each of the constituents modeled.

5. System Resource Requirements: EXPLORE-I is coded in FORTRAN and can be run on either IBM or Univac mainframes. The model requires 44K words of core on a Univac 1110 and 220K bytes on an IBM 370. A background in computer programming, engineering and environmental modeling are useful.

6. Applications: EXPLORE-I has been used by the Environmental Protection Agency for studies of hydrodynamics of the Willamette River Basin, and it has been tested in the Detroit Reservoir. Application of EXPLORE-I is relatively inexpensive, and it can be efficiently used to find sound and economical solutions to complex water pollution problems in many different types of water systems including estuaries and bays, streams and river networks, lakes and reservoirs, and combinations of these.

7. Technical Contacts

Robert B. Ambrose, Jr.
U.S. Environmental Protection Agency
Environmental Research Laboratory
College Station Road
Athens, Georgia 30605
FTS 250-3546 COM 404/546-3546

8. References

Callaway, R. J., Byram, K.V.,and Ditsworth, G.R . "Mathematical Model of the Columbia River from the Pacific Ocean to Bonneville Dam - Part I." Federal Water Pollution Control Administration, Pacific Northwest Water Laboratory, pp. 155, November 1969.

Feigner, K. D. and Harris, H.S., "Documentation Report: FWQA Dynamic Estuary Model. " U.S. Department of the Interior, Federal Water Quality Administration, July 1970.

Metcalf & Eddy, Inc. "Storm Water Management Model." Vol. 1-4. Palo Alto, California; University of Florida, Gainesville, Florida; and Water Resources Engineers, Inc. Walnut Creek, California.

Thackston, E. L. and Krenkel, P.A., "Reaeration Predictions in Natural Streams." ASCE, Proc. Journal of the Sanitary Engineering Division, Vol. 95, No. SAI, Paper 6407, pp. 65-94, February 1969.

WATER QUALITY MODEL (HAR03)

1. Model Overview: HAR03 is a computer program for the modeling of water quality parameters in steady-state multi-dimensional natural aquatic systems. The technique underlying the program is based on the law of conservation of mass, and the program can handle up to two variables reacting in a feed forward fashion with first order kinetics. The computer program from which HAR03 evolved was developed by Hydroscience, Inc., for the Massachusetts Water Resources Commission. HAR03 utilizes a numerical solution technique to a convective-diffusion equation for mass transport including decay and source terms.

2. Functional Capabilities: HAR03 is designed to model a number of water quality parameters in a steady-state, multi-dimensional natural aquatic system. The program has been constructed with the BOD-DO deficit system in mind, but with minor modifications the program may be used to model other variables which are analogous to the BOD-DO deficit system such as chlorides, coliform bacteria, polyphosphate-orthophosphate, etc. HAR03 is capable of modeling conservative substances, single reactive substances, coupled reactive substances, additive coupled substances, estuarine coupled reactive substances, and estuarine additive coupled systems. At present the program is limited to simulating a system of up to 200 sections, where each section may have up to six interfaces. A section may have only one interface to act as a boundary.

3. Basic Assumptions: In an application of HAR03, it is assumed that the variables and parameters inputted do not vary from tidal cycle to tidal cycle. The reaction coefficients are assumed to follow first order kinetics, and each individual segment of the system is assumed to be completely mixed. An orthogonal system segmentation for multi-dimensional systems is used.

4. Input and Output: HAR03 requires a large input data base

in card image form. JCL cards are required, as are cards to describe the general system being modeled. The general system cards include data for the interface parameters, the length, depth, temperature, and volume of the system. These must be followed by specific constituent cards which include data on: the number of boundaries, B.C. concentrations, photosysnthetic rates, benthal rates and loads, and other parameters for the constituents being modeled. The geometric configuration for each section is also required, as well as CBOD and NBOD removal rates, deoxygenation rates and loads.

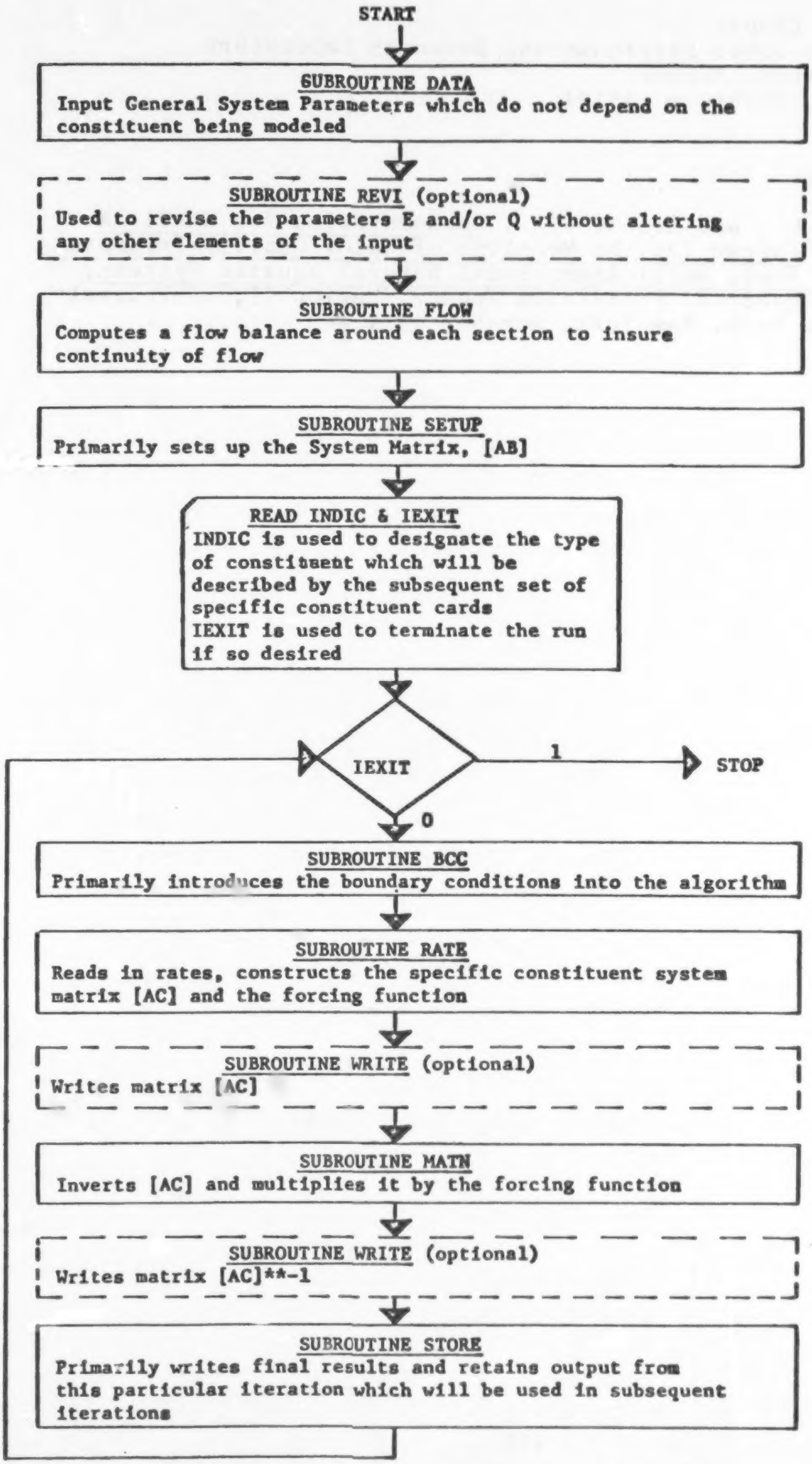
Output produced by the model includes: printouts of the input system parameters, section temperatures, volumes and depths, chloride boundary load, BOD rates and loads, correction factors, deoxygenation and reaeration rates, and BOD-DO deficits for each section in the system.

5. System Resource Requirements: HAR03 has been designed for an IBM System/370 computer, and it is written for a FORTRAN IV G or H level compiler. The program requires approximately 184K words of storage, but in order to save core storage for small systems, HAR03 has been compiled in three versions. The first version handles a system of up to 50 segments and is designated HAR50; similarly, HAR100 and HAR200 can handle a maximum of 100 and 200 segments correspondingly. The only difference between these versions is in the size of the arrays defined in the programs. A background in programming, environmental engineering and a familiarity with water quality modeling are helpful.

6. Applications: HAR03 has been used by the EPA for various applications.

7. Technical Contacts

George A. Nossa and Laura Livingston
U.S. Environmental Protection Agency
Information Systems Branch 2PM-IS
26 Federal Plaza
New York, New York 10278
FTS 264-9850 COM 212/264-9850


START
SUBROUTINE DATA
Input General System Parameters which do not depend on the constituent being modeled
SUBROUTINE REVI (optional)
Used to revise the parameters E and/or Q without altering any other elements of the input
SUBROUTINE FLOW
Computes a flow balance around each section to insure continuity of flow
SUBROUTINE SETUP
Primarily sets up the System Matrix, [AB]
READ INDIC & IEXIT
INDIC is used to designate the type of constituent which will be described by the subsequent set of specific constituent cards
IEXIT is used to terminate the run if so desired
IEXIT
1
STOP
0
SUBROUTINE BCC
Primarily introduces the boundary conditions into the algorithm
SUBROUTINE RATE
Reads in rates, constructs the specific constituent system matrix [AC] and the forcing function
SUBROUTINE WRITE (optional)
Writes matrix [AC]
SUBROUTINE MATN
Inverts [AC] and multiplies it by the forcing function
SUBROUTINE WRITE (optional)
Writes matrix [AC]**-1
SUBROUTINE STORE
Primarily writes final results and retains output from this particular iteration which will be used in subsequent iterations

FLOWCHART OF THE MAIN PROGRAM OF HAR03

Steven C. Chapra
NOAA Great Lakes Environmental Research Laboratory
2300 Washtenaw Avenue
Ann Arbor, Michigan 48104

8. References

Chapra, S.C., and Nossa, G.A., Documentation for HAR03: A Computer Program for the Modeling of Water Quality Parameters in Steady State Multi-dimensional Natural Aquatic Systems, U.S. Environmental Protection Agency, Region II, 26 Federal Plaza, New York, New York, October 1974.

WATER QUALITY MODELING SYSTEM FOR THE GREAT LAKES (WQMSGL)

1. Model Overview: The Water Quality Modeling System for the Great Lakes consists of three subsystems that allow the user to develop, calibrate, and verify water quality models for aquatic systems. Although the system was developed to serve EPA's research mandates for the Great Lakes, it has general applicability to any water system, (i.e., rivers, estuaries, small lakes, and coastal). The system can also be applied to many other water quality problems constituents, or their interactions.

2. Functional Capabilities: The functional capabilities follow:

   a) WASP - The kinetic/biochemical structures of the model are written by the user or he can apply any number of kinetic subroutines that have been developed by previous users. The transport characteristics of the water system to be modeled are assumed to be known or determined by current meter studies or hydrodynamic models. Another method of determining transport is to use WASP to trace a conservative substance through the system and adjust the transport parameters until the calculated concentration matches the measured one. WASP then numerically integrates the system mass balance equations in space and time, and calculates time variable concentrations of the substances in each special segment. A table of available kinetic subroutines, authors, capabilities, applications, and references follow. EPA and LLRS continue to support research to refine and verify these models and to incorporate new substances and processes as they are needed.

b. DASA - DASA consists of a small, working data base that is inputed directly or obtained from STORET retrievals and maintained on a DEC-PDP-11/45. A series of sub-programs are available which access the parameters under study and compute means, standard deviations, standard errors, etc. for input to MVP or for graphical display subroutines available in WASP.

c. MVP - MVP is used to make statistical comparisons between calculated concentrations and those measured. It is used during calibration to provide an efficient means to determine the difference between results of two or more "runs" which have been made varying one of the model coefficients. Finally, it can be used to judge the accuracy of the model compared to the data and to compare results of two or more models.

3. Basic Assumptions: The basic assumptions are:

a. WASP - The transport structure is known or can be determined by tracing a conservative substance. The water system can be divided into large, spacial compartments which can be assumed to be completely mixed. The time scale of the problem is on the order of weeks, seasons or decades (although smaller time scales could be considered).

b. DASA - It is assumed that data are available through a research or surveillance program over the period of time corresponding to the scale of the problem and recorded by geographical locations (station, depth), time (year, month, day, hour), and collected and analyzed according to prescribed quality control programs.

c. MVP - It is assumed that enough data exists to statistically characterize the model state variables in many of the water segments over the time scale of the problem.

4. Input and Output: The inputs for WQMSGL are:

   a. WASP - The physical characteristics of the water body, material loads, environmental factors affecting the system variables (i.e. sunlight intensity and temperature), boundary conditions, initial conditions, and model coefficients (i.e. growth rates, degradation rates, etc.)

   b. DASA - The concentration or other appropriate units connected with measurements made are input directly from terminal or cards or from direct link to STORET.

   c. MVP - The mean, standard deviation, and number for each model constituent-segment-cruise combination are received from DASA or input directly to output files from WASP of the calculated concentrations-segment-cruise combination corresponding to field measurements.

The output for WQMSGL are :

a. Output - The concentration of each state variable in each model segment at any time increment desired can be specified by the user.

b. Output - Output includes data sets in WASP graphics or MVP input formats; printouts of seasonal or cruise statistics; spatial plots of concentrations at measurement points; histograms; raw data versus time; mean and standard deviation versus time; and regression of two parameters.

c. Output:
1) Relative error model compared to data
2) T-statistics for model versus data
3) Regression statistics for model versus data

5. System Resource Requirements: WQMSGL is written in FORTRAN. It is run on DEC-PDP-11/45 or IBM 370/168. The model uses 2000 blocks of disk storage for execution. It uses a regular printer for output. A background in programming, engineering, biochemistry, and limnology is useful.

6. Applications:

WASP kinetic subroutines and applications:

Name	Summary
LAKE 1	An Eutrophication Model, developed for Lake Ontario for three vertical layers, and also applied to Lake Michigan and Saginaw Bay. State variables include phytoplankton, chlorophyll, zooplankton, carbon, three forms of nitrogen, sampling organics, and available phosphorus. References: Thomann, R.V., DiToro, D. M., Winfield, R. P., and O'Connor, D. J. Mathematical Modeling of Phytoplankton in Lake Ontario, Vol. 1: Model Development and Verification. U.S. Environmental Protection Agency, Corvallis, Oregon, 660/3-75-005, March 1975.

LAKE 1	Thomann, R. V., Winfield, R. P., DiToro, D. M., and O'Connor, D. J. *Mathematical Modeling of Phytoplankton in Lake Ontario, Vol. 2: Simulations Using LAKE-I Model*. U.S. Environmental Protection Agency, Duluth, Minnesota. In press.
LAKE III	A three dimensional, 67-segment version of LAKE-1 used for Lake Ontario.
HURO1	A refined version of LAKE-1 applied to five segments of Lake Huron with improved nutrient recycle kinetics. References: DiToro, D.M. *et al*. 1980. *Mathematical Models of Water Quality in Large Lakes; Part 1: Lake Huron and Saginaw Bay*. EPA Ecological Series. In press.
ERO1	A major revision made to Lake 1 and applied to 10 segments in Lake Erie. Improved kinetics include: 1. Division of chlorophyll between diatoms and non-diatoms 2. Silica as a limiting nutrient 3. Carbon cycle and alkalinity 4. Dissolved oxygen DiToro, D.M. and Connolly, John P. 1980. *Mathematical Models of Water Quality in Large Lakes*. EPA Ecological Research Series. In press.

CONS	A simple subroutine for tracing a conservative or first order reacting substance in a system which was applied to Saginaw Bay.

7. Technical Contact

William L. Richardson
U.S. Environmental Protection Agency
Environmental Research Laboratory
9311 Groh Road
Grosse Ile, Michigan 48138
COM 313/226-7811 FTS 226-7811

8. References

DiToro, D.M., Fitzpatrick, James J., and Thomann, R.V. *Water Quality Analysis Simulation Program (WASP) and Model Verification Program (MVP) Documentation*. Hydroscience, Inc. In preparation.

Richardson, W.L., and McGunagle, K. *Data Analysis and Storage (DASA) User's Manual*. EPA, Large Lakes Research Station. In preparation.

AGRICULTURAL RUNOFF MODEL (VERSION II)
(ARM II)

1. Model Overview: The Agricultural Runoff Management Model - Version II (ARM II) is a continuous simulation model that estimates the movement and degradation of pollutants on agricultural land surfaces. The model can be used to study pollutants including pesticides, nutrients, and sediments. ARM II is an improved version of ARM I and the Pesticide Transport and Runoff (PTR) Model published in 1973. All of these models build upon the Stanford Watershed Model. The ARM II model has been tested on agricultural plots at Watkinsville, Georgia, and is currently being tested at other sites throughout the United States. The model is recommended for use to estimate pollutant loads from agricultural fields. Applications include basin planning and evaluation of pesticides being considered for registration. ARM II was developed by Hydrocomp, Incorporated, for the U. S. Environmental Protection Agency.

2. Functional Capabilities: ARM II can be used to study the impact of various land use practices on pollutant loading to streams in agricultural areas. It can also be used to evaluate loadings of pesticides based on the physio-chemical properties of pesticides, recommended application rates, and topographical, soil, and meteorological properties of an area in which the pesticides are to be used.

For the best results, land areas simulated should not be larger then 2 mi^2. Channel processes affect timing of loadings for areas larger than this. Consequently, for areas larger than 2 mi^2, it is recommended that ARM II be used with a compatible channel routing model to insure accurate representation of significant transport processes.

The model outputs include a continuous recording of the following parameters:

1) Volume flow rate of surface runoff
2) Volume flow rate of interflow
3) Volume flow rate of base flow
4) Volume of water contained in interception storage
5) Volume of water in upper zone soils
6) Volume of water in lower zone soil
7) Volume of water in active groundwater storage
8) Rate of evapotranspiration water from land surface
9) Soil surface temperature
10) Upper zone soil temperature
11) Mass of pesticide on the watershed
12) Mass loading of pesticide
13) Concentration of dissolved pesticide in runoff
14) Concentration of adsorbed pesticide in runoff
15) Amount of pesticide degraded and volatilized
16) Amount of organic nitrogen in the soil
17) Amount of dissolved ammonia in the soil
18) Amount of adsorbed ammonia in the soil
19) Amount of dissolved nitrite plus nitrate in the soil
20) Amount of nitrogen incorporated into plant material
21) Load of organic nitrogen in runoff
22) Load of adsorbed ammonia in runoff
23) Load of dissolved ammonia in runoff
24) Load of nitrite plus nitrate in runoff
25) Concentration of dissolved inorganic phosphorus in soil
26) Concentration of adsorbed inorganic phosphorus in soil
27) Concentration of organic phosphorus in soil and
28) Amount of phosphorus incorporated into plant material

ARM II is composed of six subroutines: MAIN, LANDS, SEDT, ADSRB, DEGRAD, and NUTRNT. MAIN calls and executes the other subroutines and establishes input and output files, LANDS performs the moisture balance in the soil and generates runoff. SEDT generates and transports sediment loads. ADSRB partitions pesticides between adsorbed and dissolved phases. DEGRAD degrades pesticides contained on the soil surface. NUTRNT transforms nutrients to various forms and also establishes the equilibrium between adsorbed and dissolved phases. The model is capable of simulating changes in any parameter on 5- and 15-minute intervals. Several output formats can be selected to display results on 5-minute, 15-minute, hourly, daily, or monthly intervals. Simulations can be run for any number of years desired.

3. Basic Assumptions: Both water and pollutant transport and transformation descriptions used in the model are based on the principle of conservation of mass. Movement of water through the soil from surface to groundwater is modeled empirically. A key assumption in the model is that runoff water form the watershed simulated is derived from all locations within the watershed. Thus, it is impossible to identify the specific location as the source of a fractional load of the watershed. Degradation kinetics are also modeled empirically. All pollutant transformations are approximated by a series of first-order rate expressions. Volatilization is lumped with chemical and microbial degradation to form one rate expression for the removal and degradation of pesticides in the soil. Arrhenius equation corrections of specific transformation rate coefficients are assumed to adequately approximate temperature effects on nutrient cycling in soils. Detachment of sediment particles from the soil and transport of these particles across the watershed are empirically modeled. Pollutants are assumed to partition between adsorbed and dissolved phases instanteously.

4. Input and Output; Rainfall records.

Inputs include;

1) Control parameters that specify amount of information printed as output, operations as to whether nutrient cycles and pesticide dynamics.or just pesticide dynamics are to be simulated and definition of the period to be simulated.
2) Hydrology parameters that specify rates of water movement and nominal soil moisture storage capacity parameters.
3) Snowmelt parameters that specify snowmelt rates and snowpack characteristics.
4) Sediment parameters that define soil properties which determine sediment load response to rainfall events.
5) Pesticide parameters that determine rates of degradation of pesticides in soil, and adsorption partition between soil and dissolved phases.
6) Soil parameters that define topographical characteristics of the land surface and soil properties.
7) Nutrient parameters that define the timing and amount of fertilizer application and calculation time intervals for nutrient transformations.
8) Nitrogen and phosphorus parameters that define reaction rates and nutrient storage.
9) Chloride storage parameter.

Outputs produced by the model include an echo of the input data set, the concentration on pestides and nutrients in the soil and runoff, and loads of nutrients, pesticides, and sediment in runoff. Nutrient concentrations are reported in terms of the various forms present in the cycle. For both pesticides and nutrients, concentrations and loads for dissolved and suspended materials are reported separately. Some selection is available as to the frequency of printout. Monthly and yearly summaries for loads are also provided.

5. Systems Resource Requirements: On the IBM 370/168, using the FORTRAN H compiler, the program requires approximately 360K bytes (90,000 words) of storage for compilation of the largest subroutine. Program execution requires up to 230K bytes (57,500 words) of storage depending on the model operation selected. Thus, a computer with relatively large storage capability is usually needed for use of the ARM model. However, Version II of the ARM model has been adapted and run on a Hewlett-Packard 3000 Series II computer, which is a relatively small computer. The effort and model changes needed to adapt the ARM model to other computers will depend on the specific computer installation.

The ARM model requires no special external storage devices (tape, disc, etc.) other than the standard card reader input and line printer output. However, the model includes an option to output simulated runoff and sediment values to an external storage device as unformatted FORTRAN records.

6. Applications: ARM II has been used by the U. S. Environmental Protection Agency to evaluate potential runoff of a pesticide from agricultural lands. Application of ARM includes evaluation of best management practices for agricultural lands in relation to basin planning. It can also be used to evaluate pesticide loading in relation to registration of pesticides.

7. Technical Contacts

Lee A. Mulkey
U.S. Environmental Protection Agency
Environmental Research Laboratory
College Station Road
Athens, Georgia 30605
FTS 250-3581 COM 404/546-3581

8. References

Crawford, N. H. and Donigian, A. S., Jr., "Pesticide Transport and Runoff Model for Agricultural Lands." Office of Research and Development, U. S. Environmental Protection Agency, Washington, DC, EPA-660/2-74-013, 1973.

Donigian, A. S., Jr. and Crawford, N. H. "Modeling Pesticides and Nutrients on Agricultural Lands." Environmental Research Laboratory, U. S. Environmental Protection Agency, Athens. Georgia, EPA-600/2-76-043, 1976.

Donigian, A. S., Jr., Beyerlein, D. C., Davis, H. H., Jr., and Crawford, N.H. "Agricultural Runoff Management (ARM) Model - Version II, Refinement and Testing ." Environmental Research Laboratory, U. S. Environmental Protection Agency, Athens, Georgia, EPA-600/3-77-098, 1977.

Donigian, A.S. Jr., and Davis, H. H., Jr. "Agricultural Runoff Management (ARM) Model User's Manual: Versions I and II." Environmental Research Laboratory, U. S. Environmental Protection Agency, Athens, Georgia, EPA-600/3-78-080, 1978.

AGRICULTURAL WATERSHED RUNOFF MODEL (AGRUN)

1. Model Overview: The AGRUN model is a modification of the EPA Stormwater Management Model (SWMM) that dynamically simulates hydrology and channel pollutant loads for agricultural watersheds. This model can simulate storm runoff hydrographs and pollutographs for conservative water quality constituents which include: total suspended solids, non-settleable suspended solids, TDS, BOD, COD, chlorides, SO_4, grease, total coliforms, fecal coliforms, NH_3, organic nitrogen, nitrite and nitrate, phosphate, orthophosphate, mercury, copper, zinc, lead, chromium, cadmium, and arsenic. AGRUN is one module of a larger set of compatible programs which include a runoff model (AGRUN), a transport model, and a receiving model, and AGRUN has an interface subroutine to connect it with the other two. This model uses the Universal Soil Loss Equation to compute the suspended solids source loading rates, and it assumes that there is no decay of BOD or conversion of nitrogen forms.

2. Functional Capabilities: The Agricultural Watershed Runoff Model has the capability to simulate storm runoff hydrographs and pollutographs for up to 22 water quality parameters from agricultural watersheds. The watershed may be subdivided into as many as 200 subareas, and up to two crop types from a list of five may be specified for each subarea. Crop types include corn, beans, pasture, oats, and hay.

The tributary drainage system may be subdivided into as many as 200 channels, and the system must be dendritic in form. Cross sections may be triangular, trapezoidal, or rectangular in shape. The user has the option of representing infiltration by the Horton equation alone, in which case interflow computations are neglected, or he may specify the additional data which will be used to compute the contribution of interflow to storm runoff.

Computations of water quality can be made for up to 22 conservative constituents whose number is specified by the user. Constituents modeled include: total suspended solids, non-settleable suspended solids, TDS, BOD, COD, chlorides, SO_4, grease, total coliforms, fecal coliforms, NH_3, organic nitrogen, nitrite and nitrate, phosphate, orthophosphate, mercury, copper, zinc, lead, chromium, cadmium, and arsenic. Only total suspended solids, BOD, and fecal coliforms have been calibrated for this model. AGRUN has been used to simulate the surface runoff hydrograph for both urban and agricultural watersheds, and because it assumes no decay of BOD or conversion of nitrogen forms, the model should be considered for relatively short-term storm episodes only.

3. Basic Assumptions: The AGRUN model uses the Universal Soil Loss Equation to compute the suspended solids source loading rates, and Horton's equation to compute infiltration rates. An iterative Newton-Raphson technique is the basis for the determination of water depth and outflow rates. Velocity computations are made on the basis that flow only occurs when the soil is above field capacity. The model assumes that there is no decay of BOD and that there is no conversion of nitrogen forms.

4. Input and Output: The Agricultural Watershed Runoff Model requires a large card-image input data base. Input data for the model fall into seven categories, and these are: 1) input and program control data, 2) precipitation data, 3) drainage channel specifications, 4) land use hydrogeometric data, 5) watershed specifications, 6) soil characteristics, and 7) output control information.

For each watershed subarea, the surface area, width, and slope must be specified. For each land use type specified for each subarea, the Manning n, surface depression storage, and Horton infiltration coefficients must be entered as input data. Drainage channel specifications must include the length, invert slope, and Manning n, plus the appropriate cross section data.

If the user wishes to specify the additional data which will be used to compute the contribution of interflow to storm runoff, rather than by representing infiltration by the Horton equation alone, the following data are required for each subarea: 1) number of soil layers above the groundwater table, 2) depth of each soil layer, 3) soil permeability coefficient, 4) soil field capacity, 5) soil saturation level, 6) present field capacity available at the beginning of the storm, and 7) constant baseflow from the watershed. Constituents must be specified by the user.

Output produced by the model includes a print-out of the input data, rainfall hyetographs, runoff hyetographs, and a variety of charts representing the concentrations of the constituents.

5. System Resource Requirements: AGRUN is written in FORTRAN, and currently resides on an Univac 1108. It requires 520K bytes of core memory and a 120 character per line printer. Operators with skills in programming and engineering are useful.

6. Applications: The Agricultural Watershed Runoff Model has been used by the EPA for the Iowa and Cedar River Basins Model Project. The model was applied to the 2800-acre Buffalo Bill Watershed for four storms monitored in 1973, and it was calibrated for three parameters (suspended solids, BOD, and fecal coliforms). All subsequent simulations were performed with no adjustments in model coefficients. The model has found other applications by other users.

7. Technical Contact

Dr. Larry Roesner
Camp, Dresser & McKee, Inc.
7620 Little River Turnpike
Annandale, VA 22003
COM 703/642-5500

8. References

Roesner, L.A., Zison, S.W., Monser, J.R., and Lyons, T.C., Agricultural Watershed Runoff Model for the Iowa-Cedar River Basins, prepared for the Environmental Protection Agency, Systems Development Branch, Washington, D.C., by Water Resources Engineers, Inc., under contract No. 68-01-0742, November 1975.

NONPOINT SOURCE POLLUTANT LOADING MODEL (NPS)

1. **Model Overview**: The Nonpoint Source Pollutant Loading (NPS) Model is a continuous simulation model which estimates the movement of pollutants on land surfaces. The model can be used to study pollutants that are conserved or which degrade slowly. The NPS model is one of a series, including the Agricultural Runoff Management Model (ARM) and the Pesticide Transport and Runoff Model (PTR), which are based on the Standford Watershed Model. The model was initially tested on three predominantly urban sites and has been used in relation to planning required under Section 208 of Public Law 92-500.

The model is recommended for use to estimate nonpoint source pollutant loads in urban and rural areas. Applications are primarily waste allocation in relation to basin planning. NPS was developed by Hydrocomp, Incorporated, for the U.S Environmental Protection Agency.

2. **Functional Capabilities**: NPS can be used to study the impact of various land management strategies on pollutant loading to streams in a planning area. For best results, land areas simulated should not be larger than 2 mi^2. Since channel processes affect timing of loadings for areas larger than 2 mi^2, it is recommended that NPS be used with a compatible channel routing model to insure accurate representation of significant transport processes for areas of application larger than 2 mi^2.

The model outputs include a continuous recording of the following parameters:

1) Runoff flow rate.
2) Runoff temperature.
3) Dissolved oxygen concentration of runoff.

4) Amount of pollutant load in a given time interval for up to five pollutants.
5) Concentration of up to five pollutants in runoff.
6) Amount of sediment load in a given time interval.
7) Concentration of sediment in runoff.

NPS is composed of three major components: MAIN, LANDS, and QUAL. MAIN calls and executes the two major subroutines in the program and establishes input and output files. LANDS performs the moisture balance and generates runoff. QUAL executes erosion calculations that generate sediment loads and sediment concentration in runoff. It also calculates pollutant loads and concentrations by relating these parameters to sediment load and concentration. The model is capable of simulating changes in any parameter on 15-minute or hourly intervals. Several output formats can be selected to display 15-minute, hourly, daily, or monthly intervals. Simulations can be run for any number of years desired.

3. Basic Assumptions: Both water and pollutant transport descriptions are based on the principle of conservation of mass. The overall model is based on the Stanford Watershed Model. Water transported out of the watershed is assumed to be drawn from every portion of the watershed. Consequently, water and chemical constituents in runoff cannot be identified with any particular location within the watershed. The water balance calculations assumes that there are five water storage zones, namely, interception storage, upper zone storage, lower zone storage, active groundwater storage, and inactive ground-water storage. During a storm event, rainfall is partitioned between these storages and also exported from the watershed by overland flow, interflow and baseflow. Between storm events, export continues along with transfers between compartments. In addition, water is lost by evapotranspiration. Snow accumulation and melt is also modeled.

The rates of water export and intercompartment transfers are governed by empirical equations which contain constants requiring calibration for each application of the model. Where possible, guidance has been provided to show reasonable parameter estimates in various parts of the country. Calibration requires simultaneous rainfall and runoff records.

Sediment loss from pervious surfaces are modeled in identical fashion as the ARM Version I model. Two processes are described: detachment of fines and transport of fines. For impervious surfaces, sediment particulate accumulates and is removed according to impirical equations during dry weather periods. During storms, transport of sediment particles are defined by the same relationship as for sediment fines from pervious surfaces.

Conservative constituent transport is assumed to move at a rate proportional to the rate of movement of sediment.

4. Input and Output: The Input parameter list includes the following:

1) A set of control parameter values that defines frequency of printing of output, dates of simulation, and whether snowmelt calculations are to be performed.
2) A set of hydrology parameter values that specify the nominal capacity of the storage zone and specific rates of water transport between zones and the rates of export of water by runoff and evapotranspiration.
3) A set of parameter values that define snow pack characteristics.
4) A set of parameter values that define sediment transport characteristics.
5) A set of parameters that defines land use characteristics and for impervious surfaces, sediment accumulation, and removal rates during dry weather periods.
6) Precipitation date for period of simulation.

Outputs commonly displayed are hydrographs for each storm as well as base flow projected for dry weather periods, sediment loads and concentrations as a function of time, pollutant loads and concentrations as a function of time , dissolved oxygen concentration and temperature as a function of time. An echo of the input data set is also printed along with storm, monthly, and annual summaries of the output data sets.

5. System Resource Requirements: The NPS Model is written in the IBM FORTRAN IV language. The "handy minimal language" concept was adopted to the extent possible to produce a reasonably compatible computer code for at least the following computer systems: IBM 360, Univac 1108, CDC 6000, and Honeywell Series 32. However, at the present time, model operation has been limited to the IBM systems. The NPS model operates most effeciently in a two-step procedure. The first step involves the compilation of the program and the storage of the compiled version on disk or magnetic tape. In the second step, the compiled model is provided the necessary input data and is executed. Thus, the model can operate a number of types of different input data with a single compilation.

6. Applications: NPS has been applied to small urban watersheds in Durham, North Carolina; Madison, Wisconsin; and Seattle, Washington. It is also being used in conjunction with implementation of several 208 plans, including the plan being developed by the Northern Virginia Planning Commission.

7. Technical Contact

Lee A. Mulkey
U.S. Environmental Protection Agency
Environmental Research Laboratory
College Station Road
Athens, Georgia 30605
FTS 250-3581 COM 404/546-3581

8. References

Donigian, A. S., Jr., and Crawford, N. H. "Modeling Pesticides and Nutrients on Agricultural Lands." U. S. Environmental Protection Agency, Environmental Research Laboratory, Athens, Georgia, EPA-600/2-76-043, 317 p., 1976.

Donigian, A. S., Jr., and Crawford, N. H. "Modeling Nonpoint Pollution from the Land Surface," U. S. Environmental Protection Agency, Environmental Research Laboratory, Athens, Georgia, EPA-600/3-76-083, 280 p., 1976.

ONE-DIMENSIONAL GROUNDWATER MASS TRANSPORT MODEL (GWMTM1)

1. Model Overview: GWMTM1 is a deterministic, one-dimensional, unsteady-state, analytical model which simulates constituent concentrations in groundwater systems. It is based on the convective-dispersive mass transport equation modified for first order decay. The analytical solution is based on a semi-infinite medium with the following surface boundary condition: $C = C_o \exp(-\gamma t)$; this allows the surface concentration to be constant or exponentially varying (e.g., through dilution processes). It is typically applied in cases of vertical infiltration of wastewaters. The soil may be saturated or unsaturated (provided the moisture content is constant); the vertical seepage velocity must be constant.

2. Functional Capabilities: The program is user-oriented requiring no previous FORTRAN experience. Its digital output is in matrix form giving concentration versus distance at given times or concentration versus time at given distances. It accounts for advection, dispersion and first order decay.

3. Basic Assumptions: The model assumes a homogeneous soil and a constant seepage velocity. The constant seepage velocity requirement is met under steady, saturated conditions or steady, constant moisture content, unsaturated conditions.

4. Input and Output: Data is inputted as FORTRAN statements. The model requires only four pieces of data: the dispersion coefficient, the kinetic decay constant, the seepage velocity, and the surface constant (if the surface concentration is not constant). Concentrations are printed out at any number of specified (read in as data cards) space and time positions. It is a very simple model to operate.

5. System Resource Requirements: The model is written in standard FORTRAN IV and has been run on a S/360/91; it should run on any standard digital computer. The program requires a region size of approximately 100 K on the S/360/91. One can learn to run the model in less than a half hour and only four FORTRAN statements need to be punched (space and time positions are specified as data cards). Set up time is insignificant and FORTRAN programming knowledge is unnecessary. It has also been run on minicomputers using less than 100K of core.

6. Applications: The model was developed for the Nassau-Suffolk Regional Planning Board (Lee Koppelman, Executive Director) as part of a large 208 project. It was applied to wastewater recharge basins where the depth to water was about 30 feet. It has been distributed widely through short courses dealing with groundwater pollution and has found similar applications throughout the country.

7. Technical Contacts:

Professor Robert W. Cleary
P.O. Box 2010
Princeton, New Jersey 08540

8. References

Cleary, R.W., Final 208 Report to the Naussau-Suffolk Regional Planning Board, Hauppauge, New York, December 1977.

STORAGE, TREATMENT, OVERFLOW, RUNOFF MODEL (STORM)

1. Model Overview: The Storage, Treatment, Overflow, Runoff Model(STORM) is a continuous simulation model that provides an analysis of the quantity and quality of runoff from urban or nonurban watersheds. STORM computes loads and concentrations of six basic water quality parameters and land surface erosion. The purpose of the program is to aid in the sizing of storage and treatment facilities so that the quantity and quality of storm water runoff and land surface erosion may be controlled. The original version of the model was completed in January 1973 by Water Resources Engineers, Inc. of Walnut Creek, California, for the Hydrologic Engineering Center (HEC) and the Environmental Protection Agency. Major additions since then include the ability to compute (or specify) the quantity and quality of dry weather flow. The program and its usage are described in the current HEC STORM User's Manual dated August 19, 1980.

2. Functional Capabilities: STORM provides a means for analysis of the quantity and quality of runoff from urban and nonurban watersheds. The purpose of this analysis is to aid in the sizing of storage and treatment facilities so that the quantity and quality of storm water runoff and land surface erosion may be controlled. The model considers the interaction of seven storm water elements (rainfall/snowmelt runoff, dry weather flow, pollutant accumulation, washoff, land surface erosion, treatment rates, and detention reservoir storage). STORM computes land surface erosion and loads and concentrations of six basic water quality parameters (suspended and settleable solids, biochemical oxygen demand, total nitrogen, orthophosphate, and total coliform bacteria).

The program is designed for period of record analysis using continuous hourly precipitation data. It is a continuous simulation model that may also be used for single events. The HEC revised the input and output formats of the program to conform to standardized methods. It made program modifications which include a soil conservation service runoff curve number technique, the use of hydrographs to define runoff, pollutant accumulation in terms of pounds/acre/day, the ability to compute or specify quantity and quality of dry weather flow, specification of up to twenty land uses, and the choice of English or Metric units.

3. Basic Assumptions: The model assumes that precipitation cannot be considered without the system, and a design storm can not be defined by itself, but must be defined in the light of the characteristics of the storm water facilities. The approach used in the STORM model recognizes not only the properties of storm duration and intensity, but also storm spacing and the storage capacity of the storm water system. In this approach, rainfall washes dust , dirt, and the associated pollutants off the watershed. The resulting runoff is routed to the treatment-storage facilities where runoff greater than the treatment rate is stored for treatment at a later time.

If storage is exceeded, the untreated excess is wasted through overflow directly into the receiving waters. The magnitude and frequency of these overflows are important in a storm water study, so STORM provides statistical information on washoff, as well as overflows. The quantity, quality, and number of overflows are treated as functions of hydrologic characteristics, land use, treatment rate, and storage capacity.

4. Input and Output: Input to the model include: job specifications, hourly precipitation record, daily temperature record,

land use data including runoff parameters, pollutant accumulation and washoff data, and land surface erosion data. The hourly precipitation record and the daily temperature record are available on magnetic tape from the National Weather Service, Asheville, North Carolina.

The two main types of output are statistical information on the quantity and quality of washoff and overflow, and pollutographs for selected individual events. The STORM program produces four output reports: quantity analysis, quality analysis, pollutograph analysis and land surface erosion analysis. Input variables allow control of the level of printout which may be summary only, all events, and/or detailed analysis of selected events. The quantity and quality reports also include average annual statistics of the rainfall/snowmelt; runoff; pollutant washoff; and the quantity, quality, and frequency of overflows to the receiving water. The land surface erosion report shows average annual values for sediment production and delivery to the receiving system.

5. System Resource Requirements: The STORM program is operable on the CDC, Univac, IBM, and certain other computer systems. It requires about 50,000 words of core storage. Input is accomplished by card reader and/or a tape/disk. Output is accomplished by a 132 position line printer. Five additional tape/disk units are required for temporary storage during processing, although all five may not be used during any given run depending on input/output options. The only non-standard features of the three computer systems required by this model are those due to end of file checks and the way in which multiple output files are handled. Up to three output files are generated on tape/disk which are automatically printed at the conclusion of the job. A computer programmer to implement the program on a computer and a hydrologic and/or environmental engineer with experience in computer simulation to perform the analysis are helpful.

6. Applications: This model provides a means for analysis of the quantity and quality of runoff from urban and nonurban watersheds. The purpose of this analysis is to aid in the sizing of storage and treatment facilities so that the quantity and quality of storm water runoff and land surface erosion may be controlled. STORM has been widely used by the Hydrologic Engineering Center of the U.S. Army Corps of Engineers and by the Environmental Protection Agency.

7. Technical Contacts

Arlen Feldman
Hydrologic Engineer Center
U.S. Army Corps of Engineers
609 Second Street
Davis, CA 95616
FTS 448-2329 COM 916/440-2329

Tom Barnwell
U.S. Environmental Protection Agency
Environmental Research Laboratory
College Station Road
Athens, GA 30605
COM 404/546-3585 FTS 250-3585

8. References

Abbott, J.W., "Guidelines for Calibration and Application of the STORM Model," The Hydrologic Engineering Center, U.S. Army Corps of Engineers, Davis, California, March 1976.

American Public Works Association, "Water Pollution Aspects of Urban Runoff," Water Pollution Control Research Series, Federal Water Pollution Control Administration, Report No. WP-20-15, January 1969.

American Society of Civil Engineers, Design and Construction of Sanitary and Storm Sewers, New York, 1970.

Brandt, G.H., et al., "An Economic Analysis of Erosion and Sediment Control Measures for Watersheds Undergoing Urbanization," The Dow Chemical Company, Contract No. 14-31-0001-3392, February 1972, p. 85.

Huber, W.C., et. al., Storm Water Management Model, Users Manual, Version II, Cincinnati, Ohio, National Environmental Research Center, March 1975.

Hydrologic Engineering Center; "Pennypark Creek Water Quality Study", Special Projects Report, No. 79-S, U.S. Army Corps of Engineers, Davis, California; November 1979

Hydrologic Engineering Center; "Storage, Treatment, Overflow, Runoff Model (STORM)", Program User's Manual; U.S. Army Corps of Engineers, Davis, California; August 1977.

Kramer, Chin, and Mayo; Water Resources Engineers, Yoder, Trotter, Orlob, and Associates, for the Seattle District U.S. Army Corps of Engineers, "Environmental Planning for the Metropolitan Area, Cedar Green River Basin, Washington, Urban Drainage Study," Appendix C Storm Water Monitoring Program, December 1974.

Metcalf & Eddy, Inc., University of Florida, Water Resources Engineers, Inc., "Storm Water Management Model," Water Pollution Control Research Series, EPA Report Nos. 11024-DOC-07/71 through 11024-DOC-10/71, July 1971.

Mockus, V., et al., U.S. Soil Conservation Service, "National Engineering Handbook, Section 4, Hydrology," 1964, with revisions of 1969.

Renfro, G.W., "Present and Prospective Technology for Predicting Sediment Yields and Sources: Use of Erosion Equations and Sediment Delivery Ratios for Predicting Sediment Yield," Proceedings of the Sediment Yield Workshop, USDA Sedimentation Laboratory, Oxford, Mississippi, November 28-30, 1972.

Resource Analysis, Inc., Modifications to the STORM Program, January 1975.

U.S. Soil Conservation Service, Urban Hydrology for Small Watersheds, TR No. 55, January 1975.

Wischmeier, W.H., and Smith, D.D., "Rainfall Energy and Its Relationship to Soil Loss," Transactions, American Geophysical Union, Vol. 39, No. 2, April 1958.

STORM WATER MANAGEMENT MODEL (Version III) (SWMM)

1. Model Overview: The SWMM is a large FORTRAN program which models the complete urban rainfall/runoff cycle in an extremely comprehensive manner. It includes flow overland and in the sewerage system, in-line and off-line storage treatment (including costs) of stormwater flows. It also includes a receiving water module to assess water quality impacts. Program outputs consist of tables, hydrographs, and "pollutographs", which can be displayed at points within the system as well as in the receiving waters. The SWMM has had limited application to non-urban areas as well. An updated release of the Model (denoted Version III) became available in Jan. 1982.

The original SWMM was designed for single event simulation, producing detailed (i.e., short time increment) hydrographs and pollutographs for individual storm events. This capability remains, and the model has been modified so that it may run for an unlimited number of time steps, i.e., continuously. In this mode it may be used in a planning context, that is, for an overall assessment of urban runoff problems and estimates of the effectiveness and costs of abatement procedures. Tradeoffs among various control options, e.g., storage, treatment, and street sweeping, may be evaluated. Complex interactions between the meteorology, e.g., precipitation patterns, and the hydrology of an area may be simulated without resorting to average values or very simplified methods. In this manner, critical events from the long period of simulation may be selected for detailed analysis. In addition, return periods for intensity, duration, and volume (mass) of runoff (pollutant loads) may be assigned on the basis of the simulated record instead of equating them (unjustifiably) to the same statistics of rainfall record. In this manner, the critical events chosen for study may be substituted for hypothetical "design storms," the latter often being synthesized from intensity-duration-frequency curves on the basis of questionable statistical assumptions.

SWMM is run continuously using only the Runoff and Storage/Treatment blocks. Routing in TRANSPORT, EXTRAN, or RECEIV is avoided and is unnecessary for the planning purposes to which the model is applied. However, there is no limitation on the number of time steps for either EXTRAN or RECEIV. A receiving water model that will couple with either continous SWMM or STORM has been developed and documented.

2. Functional Capabilities: The SWMM consists of 7 blocks of subroutines. They are:

a. The Executive block assigns logical units (disk/tape/drum), determines the block or sequence of blocks to be executed, and, on call, produces graphs of selected results on the line printer. Thus, this Block does no computation as such, while each of the other six blocks are set up to carry through a major step in the quantity and quality computations. All access to the computational blocks and transfers between them pass through subroutine MAIN of the Executive Block. Transfers are accomplished on offline devices (disk/tape/drum) which may be saved for multiple trails or permanent record.

b. The Combine block allows manipulation of data sets (files stored on offline devices) in order to aggregate the results of previous runs for input into subsequent blocks. In this manner, large complex drainage systems may be partitioned for simulation in smaller segements.

c. The Runoff block computes the stormwater runoff and its associated pollution loadings for a given storm for each subcatchment, and stores the results in the form of hydrographs and pollutographs at the inlets to the main sewer system. Overland flow simulation is accomplished by a storage routing method using Manning's equation and the continuity equation. Overland flow does not begin until depression storages are full. Infiltration on pervious areas is computed by Horton's exponential function, and is subtracted from water depth existing on the subcatchment. Gutter flows are treated as a succession of steady-state flows, with routing accomplished using Manning's equation and the continuity equation. To use this block the user must input the rainfall hydrograph and a discretization of the drainage basin into sub-basins of constant land form characteristics. The location and characteristics of the gutters and pipes also have to be described. In addition, the user must input street cleaning frequency and catchbasin data as well as the land use and other features of the different areas of the basin.

d. The Transport block routes flow through the sewer system. Pre-storm conditions in the sewers are set up by computing dry-weather flow and infiltration, and distributing them throughout the conveyance system. The Transport Block then routes the storm runoff (as determined by the RUNOFF Block), the dry weather flow (DWF), and the water that has infiltrated into the system through the main sewer pipes, and through a maximum of two optional "internal" storage tanks.

The routing scheme is based on an implicit finite-difference solution of the Kinematic Wave equations, in which normalized values of the flow and conduit cross-sectional area are used. Wnen a pipe is flowing full and inflow exceeds outflow, the excess (surcharge) is stored at the upstream manhole. The flows are routed to a maximum of five outlet points.

This block requires that the sewer system be discretized into pipe segments of constant size, slope, and type joined by either manhole, control structures such as flow dividers, or "internal" storage tanks. An "internal" storage tank is described by its size, shape, outlet device, and unit cost. The outlet device can be either a pump specified to go on or off at a specified tank depth, a weir, or an orifice. The outlet device is used to specify the operation policy of the storage tank.

The DWF quality and quantity entering the sewer system are calculated by inputting to the model such parameters as daily and hourly pollution correction factors, land use population of the subareas, and average market value of the dwellings in a subarea. If more exact data is available, such as average BOD of flows, this can be used in place of some of the other data.

Infiltration is calculated by estimates of base dry weather, groundwater, and rainwater infiltration, and such parameters as average joint distance. The use of subroutines calculating DWF quality and infiltration is optional.

e. The EXTRAN block is an alternative to the TRANSPORT Block. It provides the user the capability to model sewer systems with extensive surcharging, backwater, flow reversal, looped sewers, and a variety of flow control devices. EXTRAN performs the same basic functions as the TRANSPORT block; however, there are three major differences:

   1. EXTRAN does not route water quality parameters.

2. EXTRAN uses a link-node conceptual representation of the transport system, totally unlike the TRANSPORT block.

3. EXTRAN includes the inertial terms of the Navier-Stokes equations in the solution, whereas TRANSPORT is based on a kinematic wave assumption.

Like TRANSPORT, EXTRAN sets up pre-storm conditions by computing DWF and infiltration and distributing them throughout the conveyance systems. It then performs flow routing, picking up the runoff results, and producing combined flow hydrographs for the total drainage basin and at selected intermediate points. EXTRAN may also be used strictly for stormwater routing with neither DWF nor infiltration.

The two programs are approximately the same length. The order of operations in both cases is similar, although the software itself is quite different. (EXTRAN is not a direct derivative of the original TRANSPORT block).

f. The Storage/Treatment block simulates the changes in the hydrographs and pollutographs of the runoff as it flows through a dry-or wet-weather storage/treatment plant containing up to five unit operations. Each unit operation may have detention on non-detention characteristics. The various units may be linked in a variety of configurations. Sludge handling may also be modeled using one or more units. Also, capital cost and O&M may be estimated for each unit.

g. The RECEIV block takes output from runoff, TRANSPORT, EXTRAN, or STORAGE/TREATMENT and computes the impact of the discharges upon the quality of the receiving water. The receiving body of water is discretized by the user to consist of a network of nodes connected by channels. An option in the program allows two parallel channels to be used between junctions to aid in simulating receiving bodies such as marshes. Each channel is of contant surface and cross-sectional area. Boundary conditions can be specified as a weir (outfall from a lake) or some tidal condition. RECEIV in Version III is uncharged from Version II.

3. Basic Assumptions: The model incorporates numerous assumptions, some implicit in the formulation chosen, such as in the Horton infiltration function, and some more explicit, such as the kinematic wave flow routing assumptions. The potential model users would be well advised to thoroughly understand the implications of these assumptions, as they strongly affect the model results, and will greatly influence the correct interpretation of model output. The assumptions are too numerous to be described here, and the user is referred to model documentation.

4. Input and Output: SWMM requires a large amount of input data, as described above. Typically, the collection and preparation of input data can consume 50% or more of modeling project resources. The various blocks of SWMM will accept input data in card-image form, or from disk or tape drives, particularly when output from one blocks input to the next.

The SWMM is designed as a "deterministic" model, in that if all input parameters are accurate, the physics of the processes are simulated sufficiently well to produce accurate results without calibration. This concept may fail in practice because the input data or the numerical methods may not be accurate enough for most real applications. Furthermore, many computational procedures within the Model are based upon limited data themselves. For instance, surface quality predictions are based almost totally on data from Chicago, and are unlikely to be of universal applicability.

As result it is essential that some local verification/calibration data be available at specific application sites to lend credibility to the prediction of any urban runoff model. These data are usually in the form of measured flows and concentrations at outfalls or combined sewer overflow locations. Note that the quality measurements without accompanying flows are of little value. The SWMM has sufficient parameters that may be "adjusted," particularly in the Runoff block, so that calibrating the Model against measured data is usually readily accomplished.

SWMM output is in the form of tables and various graphs of rainfall intensity, flow and pollutant concentration, or loads. Output can be provided for selected points within the system, as well as in the receiving waters. As implied above, successful use of the SWMM requires careful evaluation and interpertation of model results.

5. System Resource Requirements: SWMM is written in FORTRAN and can be run on any computer with more than 350 K bytes of core memory. Disk and magnetic tape storage vary with the application. The operator must have some knowledge of computer programming and engineering to successfully use this model.

6. Applications: The SWMM is perhaps the world's most widely used hydrologic model, having been extensively applied in the U.S., Canada, and 18 other foreign countries to such problems as:

a. Analysis and design of storm and combined sewer overflow pollution abatement facilities

b. Drainage design (urban area, subdivision, airports)

c. Analysis of storage/treatment alternatives

d. Evaluation of the effects of changes in population and land use

e. Design of systems to relieve surcharging and/or basement flooding

f. Analysis of sewer system performance

An active SWMM Users Group meets semi-annually, and publishes meeting proceedings which document a wide variety of applications.

SWMM is a complex model both computationally and theoretically, and a successful user must have a thorough knowledge of hydraulics, hydrology, and water pollution, together with some experience in water quality modeling.

7. Technical Contact

Tom Barnwell
U.S. Envirnomental Protection Agency
Environmental Research Laboratory
College Station Road
Athens, GA. 30613
COM 404/546-3585 FTS 250-3585

Dr. Wayne C. Huber
Department of Environmental Engineering Sciences
College of Engineering
A.P. Black Hall-Room 420
Gainsville, FL 32611
COM 904/392-0846 or 392-0840

8. References

Huber, W.C., et al., "Storm Water Management User's Manual, Version II," EPA-670/2-75-017, Enviromental Protection Agency, Cincinnati, OH, March 1975.

Huber, W.C., et al., "Storm Water Management User's Manual, Version III," (In Press), Environmental Protection Agency, Cincinnati, OH, 1982.

Medina, M.A. Jr., "Level III: Receiving Water Quality Modeling for Urban Stormwater Management," EPA 600/2-79-100, Environmental Protection Agency, Washington, D.C., August 1979.

Metcalf and Eddy, Inc., University of Florida, Water Resources Engineers, Inc., "Storm Water Management Model, Vol. I Final Report," Report 110 24 DOC 07/71, (NTIS PB 203 289), Environmental Proctection Agency, Washington, D.C., July 1971.

Roesner, L.A., Shubinski, R.P., and Aldrich, J.A., "Storm Water Management Model User's Manual, Version III: Addendum I EXTRAN." (In Press). Environmental Protection Agency, Cincinnati, OH, 1982.

Torno, H.C. (Editor), "Proceedings, Stormwater Management Model (SWMM) Users Group Meeting, January 10-11, 1980," EPA 600/9-80-017, Environmental Protection Agency, Washington, D.C., March 1980.

TWO-DIMENSIONAL GROUNDWATER MASS TRANSPORT MODEL (GWMTM2)

1. Model Overview. GWMTM2 is based on an analytical solution to the unsteady-state, convective-dispersive mass transport equation which describes the concentration distribution in two-dimensional groundwater systems. The model accounts for advection, dispersion in two dimensions, first order decay, and an exponentially decaying, Gaussian boundary condition. The model can be used as an excellent test of available two-dimensional, unsteady-state, numerical models; the degree of numerical models; and the degree of numerical dispersion and oscillations for different numerical solution schemes can be easily determined. In addition to exactly checking numerical models, this Gaussian boundary condition model is a valuable tool, in itself, for estimating the two-dimensional (areal or vertical cross-section) concentration pattern down-gradient from sanitary landfills, wastewater lagoons, or other groundwater pollution sources.

2. Functional Capabilities: The time-varying Gaussian boundary condition is general allowing any variance, peak concentration and center location. The exponential decay multiplier may be used or omitted. The groundwater aquifer can be any size.

3. Basic Assumptions: The model is applicable where there is a uni-directional, constant seepage velocity and the dispersion coefficients(longitudinal and lateral) are constants. This presumes steady, horizontal flow in the homogeneous aquifer.

4. Input and Output: System parameters are inputted as FORTRAN statements in the main program. Space and time positions where concentration predictions are desired are inputted as data cards. The program is user-oriented requiring the punching of less than 10 cards for parametric information.

5. System Resource Requirements: The model is written in standard FORTRAN IV and has been run on the IBM 360/91 computer; it will run on any standard digital computer. It requires a region size on the IBM machine of approximately 100K. One can learn to operate the model in less than a half hour. Set up time is insignificant and programming experience is necessary. It has also been run on minicomputers using less than 100K of core.

6. Applications: The model was developed for the Nassau-Suffolk Regional Planning Board (Lee Koppleman, Executive Director) as part of a large 208 project. It was applied to simulate the two-dimensional chloride distribution downgradient from the Babylon sanitary landfill. It was also used to check the numerical accuracy of several solution schemes of two-dimensional, numerical models of groundwater quality. It has been distributed widely through short courses dealing with groundwater pollution and has been used principally to simulate leachate plumes from landfills and check the accuracy of two-dimensional, numerical models.

7. Technical Contacts.

Professor Robert W. Cleary
P.O. Box 2010
Princeton, New Jersey 08540

8. References

Cleary, R.W., Final 208 Report to the Nassau-Suffolk Regional Planning Board, Hauppauge, New York, December 1977.

* U.S. GOVERNMENT PRINTING OFFICE: 1982 361-082/324